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ABSTRACT

Mechanical micro- and nano-patterning processes rely on engineering the interactions between a stamp and a substrate to accommodate surface roughness and particle defects while retaining the geometric integrity of printed features. We introduce a set of algorithms for rapidly simulating the stamp-substrate contact, and we use them to show that advantageous behavior can occur when the stamp consists of a finite-thickness layer bonded to a layer with different elastic properties. The simulations use two-dimensional load-response functions describing in discrete space the response of a stamp surface's shape to a localized unit load. These load-response functions incorporate the contributions both of local, indentation-like displacements and of plate-like bending of finite-thickness stamp layers. The algorithms solve iteratively for contact pressure distributions that, when spatially convolved with the load response, yield deformations consistent with the properties of the stamp and the substrate. We investigate three determinants of stamp performance: conformation to sinusoidal substrate topographies, distortion of material around stamp protrusions, and conformation to isolated spherical dust particles trapped between the stamp and the substrate. All simulation results are encapsulated in dimensionless models that can be applied to the efficient selection of stamp geometries, materials, and loading conditions. A particularly striking finding is that a stamp with a finite-thickness compliant coating bonded to a more rigid support can conform more closely to a trapped particle under a given load than a homogeneous stamp with the properties of the coating. This finding could be used to minimize the impact of particle defects on patterning processes.

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I. INTRODUCTION

Mechanical pattern transfer using micro- and nano-structured stamps is now widespread in the production of photonics,^{1,2} data storage arrays,³ biosensors,⁴ and many other devices. One such pattern transfer technique is nanoimprint lithography (NIL), in which a stamp mechanically deforms a thermoplastic polymer or an ultraviolet-curable resin (the resist), which will frequently then serve as a mask for reactive ion etching of the underlying material.⁵ In microcontact printing (μ CP), on the other hand, a stamp transfers what is often a self-assembled monolayer of molecules to a

target substrate.⁶ Microcontact processes have also been used to peel patterns from a deposited layer of, e.g., gold by selective rate-dependent adhesion.⁷ Depending on the application, the stamp might be the size of a single integrated circuit die, a whole wafer, or a patterned roller to process surfaces larger than a wafer.⁸

Mechanical requirements differ widely between the stamps used for NIL and for μ CP. NIL stamps need enough rigidity that the features on the stamp retain dimensional integrity, while allowing the stamp to conform to the inevitable non-flatness of the stamp and target substrate (there are

typically at least several micrometers of topographical variation across a wafer).^{9,10} In NIL, atomic-scale conformation of the stamp to the substrate is not needed *within* the individual features, because the resist flows into these nanoscale gaps and the residual layer of resist in the gap can usually be removed by plasma etching before subsequent processing. In microcontact printing, on the other hand, it is important for the individual features/protrusions on the stamp to deform enough to make intimate contact with the substrate, enabling molecular diffusion from the stamp to the substrate to occur, or allowing van der Waals forces to exert themselves at the interface to promote adhesion.⁶ Thus, the material at the surface of a μ CP stamp will generally have a lower elastic modulus than that of a typical NIL stamp.

Numerous stamp configurations are possible,¹¹ so in this paper, we describe a comprehensive approach to analyzing the deformations of stamps in which a finite-thickness surface layer of one elastic material is bonded to a thicker supporting layer of a second material. This modeling approach promises to be useful for tailoring stamp fabrication processes to specific applications.

A. Stamp design requirements

When engineering the compliance of a NIL or μ CP stamp, several competing objectives must be satisfied:

1. **Avoiding excessive distortion of individual features on the stamp.** Feature distortions may include bowing of cavity roofs, bulging of sidewalls, buckling of slender stamp protrusions, or adhesion between adjacent flexible stamp protrusions that are able to bend and make contact with each other. Buckling and adhesion dominate with high-aspect-ratio features, while cavity roof collapse is the main concern for lower-aspect-ratio features.¹² Hui *et al.*,¹³ Petrzela and Hardt,¹⁴ and Bietsch and Michel¹⁵ describe and model these failure modes in detail for monolithic elastomeric stamps.
2. **In NIL: limiting spatial variation of the residual layer thickness (RLT).** When pattern characteristics vary spatially, different parts of the stamp with different feature sizes, shapes, or areal densities will initially sink into the resist material at varying rates, resulting in spatially non-uniform RLT which impacts subsequent processing.^{16–19} The more rigid the stamp, the smaller these unwanted RLT variations will be for a given applied pressure.
3. **Limiting in-plane distortion of the stamp.** Under an applied pressure, some lateral distortions of the stamp are inevitable and cause overlay errors in multi-layer designs. McClelland *et al.* show that these distortions increase with Poisson's ratio of the stamp material and are inversely proportional to stamp's Young's modulus.²⁰ Under a 0.5 MPa load, for example, McClelland estimates that the overlay error of a 10 mm patterned region on a silica stamp can easily exceed 10 nm, which would be problematic for integrated-circuit production.

In NIL, the minimum required imprinting pressure is set by two needs: (1) to cause the resist material to flow in a

reasonable time and (2) to ensure conformation of the stamp to the substrate. The viscosity of the resist will dictate how great a pressure is needed to meet the first need. For overlay-sensitive applications, low-viscosity (<1 Pa s) photocurable resins tend to be used so that applied loads can be limited to a few tens of kPa,³ but some functional (*e.g.*, nanoparticle-laden) and thermoplastic imprintable materials may require loads of 0.5 MPa or more to replicate patterns within a reasonable time. In such cases, careful design of the stamp's compliance can ensure that the second need—that of conformability—is met without requiring excessively high loads.

4. **Enabling the stamp to conform to non-flat target substrates.** Substrates may have parasitic roughness, waviness, or bowing (*e.g.*, following imperfect chemical-mechanical planarization in the preceding processing²¹ or from epitaxial defects in the GaN/sapphire substrates used in LED manufacture.²² Usually, it is desirable to transfer a pattern to the full area of the substrate, so the stamp needs to conform enough to deliver a reasonably uniform contact pressure in spite of any surface imperfections. Simply increasing the applied pressure to force a high-modulus stamp to conform to a non-flat substrate may, however, exacerbate feature distortions or RLT variation.

Substrates may also be *intentionally* non-flat, as when imprinting nanostructures onto woven fabrics or optical fibers.²³ In these cases, the requirement is likely to be to make contact with as much of the curved surface as is needed with a large enough pressure across the contact region to transfer the pattern successfully.

5. **Compensating for non-flatness of the stamp itself.** The stamp itself will never be perfectly flat; it is typically made from a silicon or quartz wafer, or cast or molded from a wafer-based master pattern. Roughness, bowing, and waviness are therefore likely to be present in the stamp and need to be conformed to.
6. **Limiting the consequences of parasitic particles.** Even under clean-room conditions, particles will occasionally enter the region between the stamp and the substrate. Depending on the compliance of the stamp and the magnitude of the load applied to it, these particles may become lodged in or damage the stamp; additionally, the stamp will deform around them, losing contact with the target substrate within a certain radius around the particle.²⁴ Appropriate selection of stamp properties can help to limit the area of pattern destroyed around a particle.

Requirements 1, 2, and 3 (favoring more rigid stamps) appear to be in contradiction with requirements 4, 5, and 6 (favoring more compliant stamps). It may, therefore, be important to tailor the compliance of a stamp at multiple relevant length-scales: for example, if pattern variations occur over different length-scales from the parasitic roughness or waviness, it may be possible to design a stamp that suppresses unwanted RLT variation while promoting conformation to the substrate.

B. Existing approaches to tailoring stamp compliance

Here, we review the work exploiting the elastic and structural properties of single- and multi-layered stamps to accomplish feature fidelity, conformability to imperfect substrates, and acceptable overlay.

1. Single-layer stamps

In most stamp-based micro- and nano-patterning processes, the lateral length-scales of any parasitic topographies (e.g., wafer bowing, waviness, etc.) are larger than those of the individual features that need to be systematically transferred. A monolithic (single-layer) stamp with a particular thickness and elastic modulus is suitable in some of these cases because of the different contributions made by local deformations and plate-like bending. As we show in detail in this paper, local deflections dominate when the relevant lateral length-scale is smaller than about four times the stamp thickness, while bending deformations dominate at larger spatial periods. This transition in behavior can be exploited to make the stamp conform to imperfect surfaces while retaining local feature integrity.

For the bending component to make a useful contribution, the stamp needs to be loaded in a way that does not suppress the bending. One approach is to apply an elevated gas pressure to the back of the stamp, as Gao, Chou, *et al.* demonstrate.^{9,25,26} That approach has been implemented in NIL machines manufactured by Nanonex,²⁷ NIL Technology,²⁸ Obducat,^{29–31} among others. Equivalently, the substrate rather than the stamp can be enabled to bend—as in Wu's pneumatically-loaded wafer-bowing approach³²—or both stamp and substrate can bend together.

Bending compliance can be further enhanced by etching grooves, or flexures, into the backside of a wafer-sized stamp, as proposed by Nielsen *et al.*,^{33,34} These grooves have been found to enhance stamp bending over length-scales larger than the spacing of the grooves¹⁰ and hence could be useful to decouple adjacent chip-sized patterns mechanically on a stamp.

An alternative to pneumatic loading is to transmit the load through a soft cushion layer. Hiroshima achieves conformation of a silicon substrate to a rigid, chip-sized mold with a “sample-on-flexible-thruster” (SOFT) stage, in which an elastomeric cushion layer makes contact with the back-side of the substrate, enabling it to achieve parallelism with the mold and also to bend slightly.³⁵ In Hiroshima's experiments, the use of the elastomeric cushion was verified to deliver greater stamp-wafer pressure uniformity than a stiffer, fluoropolymer support layer. Similarly, McClelland *et al.* demonstrate the use of flexible glass ($E \approx 70$ GPa; thickness 0.15 mm) and acrylic ($E \approx 1.5$ GPa; thickness 1.2 mm) stamps, loaded via a soft cushion, to imprint bit patterns for hard disk drives.²⁰

The stamps described above vary from $\sim 100\ \mu\text{m}$ to more than 1 mm in thickness and are made from elastomers, polymers, glass, silicon, and metals—i.e., with elastic moduli spanning at least five orders of magnitude. The range of mechanical compliances that are practically achievable even with a single layer of material is enormous.

2. Multi-layer stamps

Nevertheless, parasitic surface topographies frequently occur with lateral length-scales smaller than a few hundred micrometers. For the bending of a monolithic stamp to accommodate such topographies, its thickness would probably need to be reduced below $100\ \mu\text{m}$, which would likely render the stamp fragile and difficult to handle. As a result, a range of multi-layered stamps have been developed that typically incorporate a sub- $100\ \mu\text{m}$, bendable layer of a relatively high-modulus material that carries the features and is bonded to a more compliant cushion layer. This bi-layer structure is often, in turn, attached to a more rigid backplane which suppresses in-plane distortions. In other words, most multi-layer stamp designs employ the basic principle that is used when a monolithic stamp is loaded via a soft cushion, but bonding the layers together enables layer thicknesses to be reduced while permitting straightforward handling of the stamp. Reducing the thickness of the bendable rigid layer also allows roughness components of any given wavelength to be conformed to with a smaller applied pressure, lowering the risk of stamp damage.

For example, Schmid and Michel³⁶ report contact-printing with a $30\ \mu\text{m}$ -thick patterned polymer layer of compression modulus ~ 1 MPa mounted to a 1 mm-thick elastomeric cushion layer (compression modulus 2 MPa) and then to a rigid quartz backplane. This configuration allowed printing with “sufficient accuracy,” but caused air to be trapped between the stamp and the substrate and made the stamp prone to damage during post-patterning separation. Odom *et al.*, building on Schmid's work, demonstrate a stamp made from a $\sim 40\ \mu\text{m}$ layer of a relatively stiff formulation of the elastomer polydimethylsiloxane (PDMS, elastic modulus ~ 9 MPa) mounted to a lower-modulus, 3 mm-thick PDMS cushion without a rigid backplane.³⁷ Odom successfully used the structure for phase-shifting photolithography down to 50 nm features, but does not address long-range pattern order, which might be a concern in the absence of a backplane. Li *et al.* adopted a similar approach of bonding elastomeric layers with differing compositions and hence differing moduli.³⁸

Li *et al.* adopted a similar stamp structure but with a different coating material: they photo-patterned a rigid epoxysilicone feature-carrying layer (thickness 300 nm, $E \approx 115$ MPa) onto a PDMS cushion layer (thickness $100\ \mu\text{m}$, $E \approx 4$ MPa) supported by a polyethylene terephthalate (PET) film (thickness $100\ \mu\text{m}$, $E \approx 4$ GPa).³⁹ Li's stamp design has been shown to conform sufficiently to imprint 500 nm-pitch gratings onto the tops of an array of 500 nm-high, $10\ \mu\text{m}$ -pitch micropillars as well as onto the trench regions separating the pillars. Meanwhile, Li *et al.* patterned a silicon-containing, photo-curable resin of thickness 100–200 nm onto a ~ 2 mm PDMS cushion and used this stamp to transfer patterns to the surface of a $125\ \mu\text{m}$ optical fiber, over an angle of 60° around the fiber.²³ Multi-layer stamps, therefore, appear to have potential to pattern curved surfaces as well as to conform to the imperfections of nominally flat surfaces.

The challenge posed by gas entrapment during contact between substrates and deformable stamps³⁶ points toward

a need for the systematic control of the stamp's motion and loading. To this end, Michel introduced a "rocker cylinder" printing tool in which a flexible stamp is mounted to a rigid curved holder and a contact is progressively made as the holder rotates.⁴⁰ Similarly, roll-to-roll and roll-to-plate imprint lithography offer controlled progression of the stamp-substrate contact region and frequently use a highly flexible polymeric film as the stamp or the substrate. In such cases, a compliant backing roller is sometimes used (e.g., the rubber roller of Mäkelä *et al.*⁴¹ to compensate for surface imperfections. Another solution is provided by "Substrate Conformal Imprint Lithography" (SCIL),⁴² in which an elastomeric stamp coating ($E \approx 10$ MPa) is fused to a more compliant cushion of elastomer ($E \approx 1$ MPa) on a sub-millimeter-thickness glass backplane ($E \approx 70$ GPa). This combination of materials is similar to that used by Schmid and Michel,³⁶ but in SCIL, gas entrapment is addressed by a propagating wave of pneumatic pressure on the backside of the stamp to control the development of the stamp-substrate contact region. SCIL has been developed and commercialized by Philips and Karl Süss and is based on the "wave printing" concept of Decre *et al.*¹² The modeling technique that we present here could be applied to optimizing all of these contact schemes.

Finally, it should be highlighted that problematic substrate roughness does not *always* have larger length-scales than the features that are to be patterned. In some microcontact printing applications, the highest priority may be to achieve atomically-close contact between the entirety of each stamp protrusion and the substrate, to enable the transfer of inks by molecular diffusion. In this case, one might place a thin elastomeric coating of a low modulus onto a more rigid structural material defining the features. An example is presented by Syms *et al.*, who sprayed a mixture of elastomeric precursors onto a micromachined silicon printing stamp, before curing the elastomeric layer in place.⁴³

C. A numerical framework for optimizing layered stamp compliance

We have previously demonstrated a computationally inexpensive approach to simulating NIL,^{44,45} in which we modeled the elastic deflections of a single-layer stamp of specified thickness and elastic modulus, loaded either hydrostatically or via a relatively rigid chuck. That model captured both plate-like and local indentation-like modes of stamp deformation, comprehensively covering all relevant length-scales, but did not allow for the many possibilities of multi-layered stamps with heterogeneous elastic properties. The work by Papenheim *et al.*, meanwhile, uses a plate-bending model to analyze the deformations of two-layer stamps with finite thickness and a relatively stiff backplane;⁴⁶ that analysis is expected to be particularly useful for conformation to surfaces with lateral length scales larger than the layer thicknesses.

In this paper, we present for the first time a comprehensive modeling framework for two-layer stamps that not only considers the contributions of bending and local deformation modes but also models the role of heterogeneous material

properties. We consider the influence of the elastic constants of both layers, as well as the thickness of the surface layer. We show how tuning these parameters can enable stamp designs that conform to rough surfaces and particles while limiting unwanted distortions of printed patterns.

II. MODELING FRAMEWORK

A. Multilayer elastic point load response

Our approach uses a spatially discretized Green's, or "kernel," function for the surface displacement of a layered elastic solid (Fig. 1). This function describes vertical surface displacements in response to unit pressure applied within one $\Delta \times \Delta$ -sized grid location. The function was presented by Nogi and Kato,⁴⁷ drawing upon the work of Cai and Bhushan.⁴⁸ This approach has the advantage over finite-element modeling that the ratio of the lateral discretization pitch, Δ , to the thickness, t_1 , of the finite-thickness elastic layer can be arbitrarily large. In a finite-element representation, in contrast, numerical considerations would place an upper practicable limit on the aspect ratio Δ/t_1 , in many cases necessitating far finer lateral discretizations than our method requires. Our approach thus enables simulations of stamp deformations over a wide range of length-scales at far lower computational cost than the finite element method.

Details of the load response function are given in Sec. S1 in the [supplementary material](#). Importantly, our implementation differs from Nogi's in that we embrace the spatial periodicity inherent in the use of the fast Fourier transform to convert from the spatial frequency to the spatial domain. This periodicity is valuable in describing the response of a stamp to periodic loading distributions, which are very common in mechanical lithography. We have confirmed the accuracy of the function by comparing its values to finite-element simulations for a wide range of geometrical parameters (Sec. S2 in the [supplementary material](#)).

B. Solving for contact pressure distribution and contact region

Our simulation algorithms compute the contact pressure distribution between the stamp and the substrate, accounting for any patterning or non-flatness of the stamp and/or substrate. Where the whole area of the stamp is in contact with the substrate and the stamp deformation is known, the pressure distribution can be found by simply deconvolving the deformation of the stamp (i.e., the negative of the non-flat topography) with the unit load response. If the stamp-substrate contact is partial, however, the pressure is found iteratively. Details of the algorithm vary with the geometrical situation being considered and are given in Sec. III.

Once a contact pressure solution has been found for a particular domain size (i.e., spatial period), contact geometry, layer thickness, and set of elastic properties, the result can readily be rendered dimensionless, enabling stamp performance to be assessed rapidly for any geometrically similar case.

FIG. 1. Nomenclature of the stamp model used. The top layer, Layer 1, with Young's modulus E_1 , Poisson's ratio ν_1 , and finite thickness t_1 , sits on the top of a much thicker layer, Layer 2, that is modeled as an elastic half-space with Young's modulus E_2 and Poisson's ratio ν_2 . Adapted from Nogi and Kato.⁴⁷

C. Other assumptions

We assume that there is no adhesion between the stamp and the substrate; hence, contact pressures are always compressive. In Secs. III A–III C, we consider stamp deflections to be much smaller than t_1 because stamp protrusions are generally much smaller than the stamp coating, and wafer/substrate roughness is generally much smaller than t_1 over length scales comparable to t_1 . In Sec. III D, we assume stamp deflections to be small when $E_1 \geq E_2$ and the bulk of the deformation can be considered to occur in the very thick layer 2; however, we do consider finite changes of the thickness of layer 1 when $E_1 < E_2$ and the stamp coating undergoes significant deformation around a particle. In all cases, deformations are modeled as purely out of the plane of the stamp (in the z direction); these displacements can include bending, transverse shear, and local indentation of the stamp material. Contact pressures are assumed not to give rise to any lateral material displacements within the (x, y) plane of the stamp surface.

We ignore any capillary pressures exerted by resist or ink on the stamp or substrate.⁴⁹ Indeed, we neglect the presence of any viscous material between the stamp and the substrate. Our rationale for this assumption is as follows. In μ CP, the ink is generally diffused into the stamp and any interfacial film of liquid can reasonably be expected to be negligible in thickness. In NIL, meanwhile, the thickness of the resist film can be considered uniform at the beginning of imprinting (e.g., having been spun onto the substrate), and therefore to have a surface topography that is no rougher than that of the substrate. At the instant immediately after the load is first applied, no resist flow can have occurred and the stamp's deformed shape is therefore well approximated as being the same as if the uniform-thickness resist film were not present.

Resist will immediately begin to flow, under load, into uncontacted regions, causing the stamp-resist contact area to grow. Our simulations will therefore, if anything, underestimate the amount of contact between the stamp and resist-coated substrate at any moment. Since a desirable outcome of the design of a stamp is to maximize the area of contacted and hence patterned regions in spite of substrate roughness or parasitic particles, our simulations can be regarded as conservative by tending to underestimate the amount of contact. The results presented here provide design guidelines, and full NIL simulations using our previously published framework for modeling resist and stamp deformation⁴⁴ would be expected to be used later, once an optimized stamp configuration has been chosen.

III. DEVELOPMENT OF REDUCED-ORDER STAMP DEFORMATION MODELS

The objective of this work is to provide a rational approach to designing NIL and μ CP stamps, enabling stamps to conform to non-flat substrates and parasitic particles while not allowing individual features on the stamps to become excessively distorted.

A. Stamp conformation to sinusoidal topographies

We begin by considering the stamp-average pressure, $p_{0,s}$, needed to force a layered stamp to conform fully to a 2-D sinusoidal topography with peak-to-peak amplitude $z_{0,s}$ and wavelength (spatial period) λ_s [Fig. 2(a)]. This topography is intended to be representative of a particular spatial frequency component of the inevitable nanoscale roughness occurring on a substrate or stamp surface.

FIG. 2. The three stamp-deformation situations considered, shown in cross-section: (a) conformation to a rigid, two-dimensional sinusoidal topography, (b) distortion of individual features (both parallel lines and cylindrical protrusions; layouts shown in plan), and (c) conformation to a spherical dust particle of radius r_0 , leaving an uncontacted region radius r_k .

We are interested in how $p_{0,s}$ depends on Young's modulus E_1 , Poisson's ratio, ν_1 , the thickness, t_1 , of the stamp's finite-thickness surface layer, and the elastic properties of the supporting half-space of material, E_2 and ν_2 . We first define one period of a 2-D sinusoidal substrate topography in discrete space, with the nominal amplitude $z_{0,s} = 1$ m, and surface positions across $M \times N$ locations as follows:

$$z_s(x_a, y_b) = z_{0,s} \sin\left(\frac{2\pi a}{M}\right) \sin\left(\frac{2\pi b}{N}\right) \quad (1)$$

for $1 \leq a \leq M$; $1 \leq b \leq N$,

where $x_a = a\Delta$, $y_b = b\Delta$, $M = N$, and $\lambda = M\Delta$. (The 1 m value of $z_{0,s}$ is arbitrarily selected; the solution obtained below for the contact pressure distribution is subsequently normalized by the nominal amplitude $z_{0,s}$, the layer elastic modulus, and the layer thickness to give a dimensionless “conformability.”)

For each combination of stamp elastic properties that we wish to consider, we generate the discrete unit load-response function in the spatial frequency domain (Sec. S1 in the [supplementary material](#)), with size $M \times N$ and zero d.c. component: $\bar{C}_0(\xi_m, \eta_n)$. We seek the pressure required for complete conformation, so we assume full contact and deconvolve $z_s(x_a, y_b)$ with the unit load response. This computation yields a pressure distribution $p_s(x_a, y_b)$ with zero mean,

$$p_s(x_a, y_b) = \text{IFFT}\left[\frac{\text{FFT}[z_s(x_a, y_b)]}{\bar{C}_0(\xi_m, \eta_n)}\right], \quad (2)$$

where $\text{FFT}[\cdot]$ and $\text{IFFT}[\cdot]$ are the 2D fast Fourier transform and its inverse, respectively. The FFT and inverse FFT operations implicitly assume spatial periodicity, so although our simulation region contains only one period of the pattern, the simulation effectively finds the pressure distribution consistent with a sinusoidal topography of infinite lateral extent.

Since we assume no adhesion between the stamp and the substrate, actual contact pressures cannot be negative. By applying a uniform pressure $p_{0,s}$ to the backside of the stamp, however, we can increase all pressures in the stamp-substrate contact region by $p_{0,s}$. Thus, the minimum applied

pressure at which conformation to the sinusoidal topography is achieved and all contact pressures are at least zero, is given by

$$p_{0,s} = -\min[p_s(x_a, y_b)] \quad \forall a, b. \quad (3)$$

We have carried out simulations spanning six orders of magnitude in λ_s/t_1 , as well as exploring the effects of the two layers' Poisson's ratios. In these simulations, $N = M = 64$, and a convergence study confirmed that finer spatial discretization did not significantly alter the results. We summarize these simulation results by plotting the dimensionless “conformability” of the stamp, $(z_{0,s}/t_1)(E_1/p_{0,s})$, against the dimensionless spatial period of the topography, λ_s/t_1 (Fig. 3). (We define conformability differently from Bietsch and Michel,¹⁵ who define it as the ratio of work of adhesion to Young's modulus of the stamp.)

For a monolithic stamp ($E_2 = E_1$), conformability is directly proportional to the spatial period: in other words, the amount of topographical variation to which a stamp can conform under a given pressure is proportional to the wavelength of the topography, with all else being equal.

Next, we consider stamps that have a finite-thickness surface layer that is stiffer than the supporting cushion of material. For topographical wavelengths much smaller than the layer thickness ($\lambda_s \ll t_1$), conformability is proportional to wavelength, just as in the monolithic stamp, because most stamp deformation is confined to the surface layer. Once the wavelength exceeds about $4t_1$, however, plate-like bending of the surface layer begins to dominate, and stamp conformability rises much more rapidly with wavelength: proportional to $(\lambda_s/t_1)^4$. As the wavelength increases still further, stresses in the supporting cushion (E_2) play an increasing role, and conformability eventually returns to a regime in which it is proportional to wavelength but $(E_2/E_1)^{-1}$ times higher than that for very small wavelengths.

Different behavior occurs when the finite-thickness surface layer has lower elastic modulus (E_1) than the supporting material (E_2). In this case, again, for very small topographical wavelengths ($\lambda_s \ll t_1$) most stamp deformation happens within the surface layer and the stamp behaves as if it were monolithic with modulus E_1 . Once the wavelength exceeds

FIG. 3. Summary of the ability of a layered stamp to conform to a rigid sinusoidal topography. The dimensionless peak topographical amplitude to which the stamp can conform (the “conformability”) is plotted against the dimensionless pitch of the topography for a range of ratios of the stamp’s backing layer modulus (E_2) to that of its finite-thickness layer (E_1). Results are shown for a range of top-layer Poisson’s ratios (ν_1). Dependence on Poisson’s ratio of the backing layer (ν_2) is relatively mild. Symbols show numerical simulation results, and lines show the model fit to these results (see Sec. III C). $N = M = 64$.

about $4t_1$, however, rather than exhibiting plate-bending as in the $E_1 > E_2$ case, the surface layer of the stamp now begins to behave as a squeezed film of material, and dimensionless conformability can actually fall with increasing topographical wavelength.

This fall in conformability occurs because of the increasing difficulty of displacing the material over greater lateral distances within the squeezed layer. The trend in conformability is highly sensitive to Poisson’s ratio of the surface layer, ν_1 . Completely incompressible layers ($\nu_1 = 0.5$) show the most severe fall in conformability, with conformability inversely proportional to the square of the wavelength. Even a small amount of compressibility, however (e.g., $\nu_1 = 0.49$), alleviates this effect considerably, and for $\nu_1 = 0.30$ —as, for example, in glassy polymers—conformability simply reaches a plateau rather than decreasing for $\lambda_s \gg t_1$. Whatever the value of ν_1 , for very high λ_s/t_1 the conformability eventually returns to being proportional to λ_s/t_1 , but (E_2/E_1) times lower than that for very small wavelengths.

We have therefore identified relationships between the dimensionless parameters $(z_{0,s}/t_1)(E_1/p_{0,s})$, (λ_s/t_1) , (E_2/E_1) , and ν_1 . We find that results are not strongly sensitive to Poisson’s ratio of the supporting material: results for values of ν_2 of 0.3 and 0.5 are shown in Fig. 3 and are virtually indistinguishable.

This analysis provides a potentially useful way to optimize the design of layered stamps to conform to topographies with known surface roughness spectra. A suggested systematic approach is to decompose the surface roughness into a finite number of spatial frequency components and design the stamp such that it can conform to each frequency component independently. Once the stamp has been designed, a simulation of its interaction with the full surface topography could be carried out to check for any unanticipated interactions between different frequency components.

It should be noted that this approach finds the value of $p_{0,s}$ needed to bring the stamp into contact with every

point of the topography. The contact pressure distribution $p_s(x_a, y_b)$ is not uniform, and in the most deeply recessed points of the sinusoidal topography, although contact is made, the contact pressure approaches zero. A user of this model needs to consider this attribute and may need to increase the average applied pressure to ensure pattern transfer at all locations. As mentioned in Sec. II C, once this framework has been used to design a stamp, a full NIL simulation⁴⁴ may be used to confirm exact process parameters.

B. Deformation of stamp features

The need to achieve conformation to non-flat substrates must be balanced with the need to maintain enough stamp rigidity to limit feature-level distortions under realistic loads. Next, we explore how the amount of vertical deflection of the roof of a stamp cavity depends on its geometry and on the compliance of the stamp.

We consider two example feature geometries: parallel ridges and cylindrical protrusions arranged in a square array [Fig. 2(b)]. The pitch of the features is defined as λ_f , and the widths of the ridges and the diameters of the cylindrical protrusions are $\lambda_f/2$. The maximum amount of vertical deflection of the cavity roof is $z_{0,f}$. In our model, only stamp protrusions make contact with the substrate, so we cannot simply deconvolve the stamp topography with a load response function; instead, we use an iterative approach, the biconjugate gradients method,⁵⁰ to find the contact pressure distribution $p_f(x_a, y_b)$ within the contact region that satisfies both equilibrium and compatibility of the contacting bodies for a nominal stamp displacement. From this pressure distribution, we compute the parasitic stamp deformations in the uncontacted regions inside the cavities. The relation that is iteratively solved for $p_f(x_a, y_b)$ is

$$z_f(x_a, y_b) = \text{IFFT}\{\overline{C_0}(\xi_m, \eta_n) \times \text{FFT}[p_f(x_a, y_b)]\}, \quad (4)$$

subject to the constraints that

$$z_f(x_a, y_b) = 1 \text{ m} \quad \forall a, b \in C, \quad (5)$$

$$p_f(x_a, y_b) = 0 \quad \forall a, b \notin C, \quad (6)$$

where C is the set of locations occupied by stamp protrusions, in which the stamp–substrate contact exists. Once this pressure distribution has been found, the corresponding surface displacements $z_f(x_a, y_b)$ within the cavity region are found by substituting the pressure solution directly into Eq. (4). The peak cavity roof displacement, $z_{0,f}$, is defined as the peak-to-peak range of $z_f(x_a, y_b)$ over all locations within the simulation region. (We assume that the height of the stamp protrusions is very small compared to t_1 , so that any reduction of the height of the protrusions is negligible. For NIL stamps, where the surface layer is typically $\sim 100 \mu\text{m}$ or more and the features are usually sub-micron in height, this is a realistic assumption, and deformations *within* individual protrusions can be expected to be around 1% of those within layer 1.)

Meanwhile, the average of the pressure across one period of the pattern—and thus also the stamp-wide average—that corresponds to a nominal displacement of 1 m in the contact region is computed as

$$p_{0,f} = \frac{1}{MN} \sum_{a=1}^M \sum_{b=1}^N p_f(x_a, y_b). \quad (7)$$

In Fig. 4, we show how the dimensionless cavity roof distortion, $(z_{0,f}/t_1)(E_1/p_{0,f})$, changes with the dimensionless feature pitch, λ_f/t_1 , over six orders of magnitude. Again, these simulations used $N=M=64$. The trends are very similar to those for the conformability of a stamp to a sinusoidal substrate (Sec. III A). For $\lambda_f \ll t_1$, feature distortion is directly proportional to the feature pitch. For $\lambda_f \gtrsim 4t_1$ and $E_1 > E_2$, plate-bending of the top stamp layer between protrusions means that dimensionless

distortion rises as $(\lambda_f/t_1)^4$, before returning to being directly proportional to λ_f/t_1 for $\lambda_f \gg t_1$. For $\lambda_f \gtrsim 4t_1$ and $E_2 > E_1$, dimensionless feature distortion $(z_{0,f}/t_1)(E_1/p_{0,f})$ actually falls with increasing λ_f/t_1 in a way that is highly sensitive to ν_1 , because of the squeezing mode of deformation of the stamp surface layer.

The constant of proportionality linking $(z_{0,f}/t_1)(E_1/p_{0,f})$ to (λ_f/t_1) is slightly more than twice as large for cylindrical protrusions as for parallel lines. This result is expected, for two reasons. Firstly, for a given λ_f , the maximum distance between two cylindrical protrusions is greater than the maximum distance between two parallel lines, enabling larger cavity roof distortions to occur between the cylindrical features. Secondly, while the parallel lines constrain stamp distortions to take place in plane-strain, the cylindrical protrusions do not. Similar relationships could readily be computed for other protrusion shapes and areal densities.

To aid in a physical understanding of the stamp distortions involved, Fig. S2 in the [supplementary material](#) shows simulations of distorted cavity roof profiles for arrays of cylindrical stamp protrusions with $0.1 \leq \lambda_f/t_1 \leq 1000$ and $10^{-3} \leq E_2/E_1 \leq 10^6$. For example, if $E_2 \gg E_1$, as λ/t_1 increases, the distorted shape of the roof transitions from being parabolic ($\lambda/t_1 = 0.1$) to having two separate locations of maximal distortion nearer to the protrusion walls ($\lambda/t_1 = 10$), to having a plug-like shape ($\lambda/t_1 = 1000$). Physical explanations of these deformation modes are discussed in Sec. S3 in the [supplementary material](#). All of the trends in roof distortions flow from the unit load response of the bilayer stamp, underlining the generality of the simulation approach.

C. A unified dimensionless model for wafer/stamp conformation and feature distortion

We find that the results of Secs. III A and III B can be integrated into a single dimensionless model with six parameters, k_0 to k_5 , whose values depend on whether

FIG. 4. Dimensionless summary of the peak deflections of the cavity roofs of imprinted features. Poisson's ratio of the backing/support material, ν_2 , was set to 0.30. A feature width-to-pitch ratio of 0.5 was used throughout. Symbols show numerical simulations and lines show the model fit in Sec. III C. $N = M = 64$.

conformation to sinusoidal topographies or feature distortion is being considered. In the relationship below, represents $z_{0,s}$ in the case of the sinusoidal topography and $z_{0,f}$ in

the case of feature distortion modeling. Similarly, p_0 represents either $p_{0,s}$ or $p_{0,f}$ and λ represents either λ_s or λ_f . The dimensionless model is

$$\frac{z_0 E_1}{p_0 t_1} = \begin{cases} k_0 \frac{\lambda}{t_1} + \left\{ \left[k_1 \left(\frac{\lambda}{t_1} \right)^4 \right]^{-1} + \left[k_0 \left(\frac{E'_1}{E'_2} \right) \left(\frac{\lambda}{t_1} \right) \right]^{-1} \right\}^{-1} & E_2 < E_1, \\ k_0 \frac{\lambda}{t_1} & E_2 = E_1, \\ \left\{ \left[k_0 \left(\frac{\lambda}{t_1} \right) \right]^{-k_3} + \left[k_2 \left(\frac{\lambda}{t_1} \right)^{-2} + F_1(v_1) + k_0 \left(\frac{E'_1}{E'_2} \right) \left(\frac{\lambda}{t_1} \right) \right]^{-k_3} \right\}^{-\left(\frac{1}{k_3} \right)} & E_2 > E_1, \end{cases} \quad (8)$$

where

$$F_1(v_1) = k_4 \left(1 - e^{-\left(\frac{0.5-v_1}{k_5} \right)} \right), \quad (9)$$

$$E'_k = \frac{E_k}{(1 - \nu_k^2)} \quad \text{for } k = 1, 2 \quad (10)$$

and the parameters k_0 to k_5 are given in Table I. This simplified algebraic relationship could be used to reduce the number of numerical simulations needed to optimize stamp properties for a given application.

For $E_2 = E_1$, the stamp deformation is simply proportional to pattern pitch. For $E_2 < E_1$, the model captures the transition of the stamp deformation from local deflections of layer 1 to plate-like bending of layer 1 as the spatial period of the pattern increases above t_1 . The plate-like bending term is proportional to $(\lambda/t_1)^4$.

For $E_2 > E_1$, the model captures the transition from local deflections of layer 1 to thin-film “squeezing” of layer 1, as the spatial period of the pattern increases above t_1 . The squeezing term is proportional to $(\lambda/t_1)^{-2}$ and corresponds to a parabolic pressure distribution beneath each period of the pattern. The

squeezing term directly governs stamp deflections when layer 1 is incompressible ($\nu_1 = 0.5$). For other values of ν_1 , the variable $F_1(v_1)$ captures the transition from pure squeezing toward a combination of squeezing and compression.

D. Stamp-substrate contact behavior around dust particles

In Secs. III A–III C, we developed a model to help us design stamps that will conform to rough substrates while limiting feature distortion of cavity rooves. Another key aspect of a stamp’s performance is how well it conforms to random *particle defects* between the stamp and the substrate. The presence of a particle will prevent complete contact between the stamp and the substrate [Fig. 2(c)], hindering uniform pattern transfer. It is desirable to minimize lost contact area by designing the stamp to conform as closely as possible to the particle. In this section, we model how layered stamps conform to a hard, spherical particle of radius r_0 resting on a rigid substrate. We simulate rigid coatings on compliant supporting layers ($E_2/E_1 < 1$) differently from compliant coatings on more rigid supports ($E_2/E_1 > 1$) because in the latter case, thickness changes of layer 1 may be large and must be accounted for, requiring a different and slightly more computationally expensive approach.

1. Stamp-particle conformation for $E_2/E_1 < 1$

Our simulations have established the relationship between the size of the non-contacted region, with “kill” radius r_k , around the particle and the stamp-average pressure (Fig. 5). Details of the algorithm are given in Sec. S4 in the [supplementary material](#).

The simulation results show that as the dimensionless applied pressure increases, r_k/r_0 asymptotically reduces toward a value of 1, which represents full envelopment of the particle by the stamp. For $t_1 \gg r_0$, the surface layer of the stamp behaves similarly to an elastic half-space from the perspective of the particle, and an inverse-square-root relationship between the average applied pressure, $p_{0,d}$, and the

TABLE I. Parameters fit for the model of stamp conformation and feature distortions.

Parameter	Conformation to sinusoidal topography ($z = z_s$)	Inter-feature cavity-roof distortion ($z = z_f$)	
		Parallel lines	Cylindrical pads
k_0	0.12	0.30	0.69
k_1	0.0011	0.0011	0.0076
k_2	48	1200	9600
k_3	0.70	0.30	0.30
k_4	0.48	1.0	2.3
k_5	0.11	0.13	0.10

FIG. 5. Dimensionless summary of the uncontacted (“killed”) radius surrounding a dust particle trapped beneath a layered stamp, as a function of layer thickness, layer elastic properties, and applied pressure. Results here are for stamps with a coating that is stiffer than the supporting base. Poisson’s ratio of layer 2 was fixed at 0.3. $N = M = 128$.

uncontacted radius, r_k , is seen until r_k becomes very close to r_0 . As t_1 falls and becomes comparable to or smaller than r_0 , however, layer 1 behaves increasingly like a bending plate on an elastic foundation. The larger the mismatch between layer moduli [e.g., Fig. 5(a), where $E_2 = 0.01E_1$], the more sensitive the r_k - $p_{0,d}$ relationship becomes to the thickness of layer 1. This phenomenon could be exploited to design stamp coatings whose material is rigid enough to limit individual feature distortions, and whose thickness is small enough to limit particle kill radii. This possibility is relevant when the features are considerably smaller than the largest parasitic particles anticipated (e.g., for NIL, 100 nm features and $1\mu\text{m}$ particles would be typical). Overall, these results indicate the potential of a rigid coating on a more compliant support to enable high-resolution patterning while remaining robust to inevitable particle defects.

Meanwhile, our choice of the dimensionless pressure axis, $p_{0,d}/[E_1/(1-\nu_1^2)]$, which normalizes the applied pressure by the plane-strain modulus of the stamp’s surface layer, appears to capture effectively the dependence of the results on ν_1 : results from both the considered values of ν_1 collapse onto a single line for any given t_1/r_0 .

Based on the simulation results, we have established the following model for the relationship between stamp properties, $p_{0,d}$ and r_k , which incorporates the half-space and plate-like bending regimes just described

$$r_k = (\{[r_P^a(E_1, \nu_1, t_1) + r_L^a(E_2, \nu_2)]^{b/a} + r_L^b(E_1, \nu_1)\}^{c/b} + r_0^c)^{1/c}. \quad (11)$$

A good fit is obtained with $a = 1.5$, $b = -3$, and $c = 1.7$. In this model, the quantity $r_L(E, \nu)$ is the uncontacted radius that would result from local material deflection of an elastic half-space

$$r_L(E, \nu) = r_0 \sqrt{\frac{E}{2(1-\nu^2)p_{0,d}}}. \quad (12)$$

Meanwhile, $r_P(E, \nu, t)$ is the uncontacted radius that would result from bending of a plate of material supported on a relatively very low-modulus material

$$r_P(E, \nu, t) = \left(\frac{128r_0D}{3p_{0,d}}\right)^{0.25}, \quad (13)$$

where D is the bending stiffness of the layer of material that is bending

$$D = \frac{Et^3}{12(1-\nu^2)}. \quad (14)$$

The model is superimposed in Fig. 5 as solid ($\nu_1 = 0.3$) and dashed ($\nu_1 = 0.49$) lines, and close correspondence is seen between the model and the numerical simulation results.

2. Stamp-particle conformation for $E_2/E_1 > 1$

In Sec. III D 1, we showed how a rigid coating on a more compliant layer could maintain the dimensional integrity of imprinted features while conforming to unwanted particles.

In other types of process, such as microcontact printing, maximizing the contact area within each feature may be a higher priority, and it may be preferable to use a thin compliant coating on a more rigid base layer.

Because much of the stamp deformation now happens in layer 1, and t_1 is not necessarily much larger than r_0 , finite thickness reductions of layer 1 around the particle need to be considered. The algorithm that we use for $E_2 > E_1$, therefore, works by gradually moving the stamp toward the substrate in a series of pre-defined displacement steps and tracking the growth of the contact region as well as the spatial and temporal evolution of the thickness of layer 1. To model the spatial variation of layer 1 while still allowing the computationally inexpensive approach of convolving pressure distributions with load response kernel functions, a thickness-binning approach is used that subdivides the layer into zones with different thicknesses and applies a separate load-response kernel in each zone. Details of the simulation algorithm for $E_2 > E_1$ are given in Sec. S5 in the [supplementary material](#).

Figure 6 summarizes the simulated effects of t_1/r_0 , E_2/E_1 , ν_1 , and ν_2 on the ability of a stamp to conform to particle defects. The performance metric reported on the vertical axes, R_p , is the ratio of the backside pressure needed to achieve $r_k = 1.35r_0$ using a layered stamp to that needed to achieve the same r_k with a thick, homogeneous stamp of Young's modulus E_1 and Poisson's ratio ν_1 . A value of $R_p < 1$ indicates that the layered stamp conforms to a particle more effectively than a homogeneous stamp. While there is nothing particularly significant about the threshold of $1.35r_0$, it is chosen because it represents a non-contacted area less than twice the projected area of the particle and would likely be considered an

acceptable level of conformation. More complete results showing relationships between r_k/r_0 and $p_{0,d}/E_1$ across the explored parameter space are shown in Fig. S4 in the [supplementary material](#).

For all values of ν_1 and E_2/E_1 considered, the minimal (i.e., optimal) value of R_p occurs for $2 \leq t_1/r_0 < 4$. Coatings that are too thin require considerable deformation of the rigid support to conform, while coatings that are too thick approach the behavior of a half-space of material. The most ideal case of all considered is $E_2/E_1 = 100$, $\nu_1 = 0.49$, and $t_1/r_0 = 2$. Here, $R_p = 0.2$, meaning that only 20% as much pressure needs to be applied to the backside of the stamp to meet the conformation threshold as would be needed with a non-layered stamp. Reducing the required pressure by such a factor could have many benefits, including a lower probability of stamp or substrate damage and less feature distortion.

The ability of a thin compliant coating on a more rigid support to yield better conformation behavior than a thicker compliant stamp might be regarded as surprising: one might imagine that the more the stamp was made from a lower-modulus material, the better it would conform. In fact, having a finite-thickness compliant coating can aid conformation by causing the compliant material to be displaced into the gap immediately around the particle rather than simply being displaced into the bulk of the stamp. As $p_{0,d}$ increases, the material from a finite-thickness layer 1 more readily touches the substrate, reducing r_k . This effect becomes more pronounced as layer 1 approaches incompressibility ($\nu_1 \rightarrow 0.5$). The effect is illustrated by the deformed stamp profiles illustrated in Fig. 7, which show how, at a chosen $p_{0,d}$, conformation is markedly better for $t_1/r_0 = 2$ than for either $t_1/r_0 = 1$ or $t_1/r_0 = 10$.

FIG. 6. Summary of how using a finite-thickness compliant stamp coating (modulus E_1) on a higher-modulus (E_2) supporting material can reduce the imprinting pressure $p_{0,d}$ needed to achieve a target kill radius r_k , compared to simply using a half-space of the same coating material. Here, R_p is the ratio of $p_{0,d}$ required to achieve $r_k = 1.35r_0$ using the layered stamp to that required for the same kill radius using a half space of the same coating material. Conformation is around a hard spherical particle of radius r_0 . Results for $\nu_2 = 0.3$ and $\nu_2 = 0.5$ are shown and indicate very weak dependence of R_p on ν_2 . $N = M = 256$.

FIG. 7. Cross-sections through the simulated surface of a layered stamp conforming to a hard spherical particle. For each value of E_2/E_1 shown, conformation results are illustrated for three values of t_1/r_0 . For a particular E_2/E_1 , all topographies are shown for $\rho_{0,d}/E_1$ equal to the value required to achieve a kill radius of $r_k = 1.35r_0$ in the case of $t_1/r_0 = 2$ (details in the [supplementary material](#)). These results illustrate that for $t_1/r_0 = 2$, a smaller kill radius can be achieved at a given applied stamp-average pressure than if the layer thickness were much larger. This result is not immediately intuitive because one might expect that the thicker the compliant coating, the more easily the kill radius would be reduced with increasing pressure. E_1 is held constant; $\nu_1 = 0.45$; $\nu_2 = 0.3$. $N = M = 256$.

The optimal result shown in [Fig. 6](#) suggests that if one can freely choose a stamp coating material, one would prefer the lowest coating modulus available and an effectively incompressible material such as an elastomer. Once the coating material has been chosen, the backing material should be chosen to have $E_2 \sim 100E_1$, which provides some additional conformability while still forcing the coating material into the gap around the particle. The value of ν_2 is found to have a very minor effect.

E. Computational cost

The use of pre-computed kernel functions to describe the load responses of multi-layered stamps enables deformation processes to be tracked with a small number of 2D matrices, rather than requiring a full 3D mesh as in finite-element simulations. A single forward convolution of a pressure distribution with a unit load response for, say, $N = M = 256$ requires ≤ 1 ms on a standard personal computer. Each solution step, however, requires multiple iterations of the biconjugate gradients algorithm and therefore many convolutions. The number of iterations needed to converge to a reasonable error depends strongly on the form of the load response function and the

fraction of the simulation region in contact. For large contact area fractions, several hundred iterations may prove necessary. Moreover, each step-change in pressure described in [Sec. III D](#) must be solved iteratively, and the number of pressure steps required for a stable solution can be in the hundreds. Therefore, the simple one-step deformations of each stamp configuration in [Secs. III A](#) and [III B](#) can be simulated within ~ 1 s, while simulating conformation to particles as described in [Sec. III D 1](#) may take a few minutes and the cases in [Sec. III D 2](#) may require 30–60 min. We explored a large range of stamp designs with a few hours of simulation time, which would be well beyond the capabilities of a conventional finite-element approach. Memory requirements are also modest, with the most demanding case in [Sec. III D 2](#) peaking at a few GB.

IV. TWO APPLICATION EXAMPLES

Finally, we show how our models can be used to design stamps for specific applications. The first case we consider is a nanoimprint lithography process in which uniform imprinting is desired across a whole silicon wafer. We have previously measured the nanoscale roughness spectra of several silicon wafers⁵¹ and found their power spectral magnitudes to be approximately proportional to wavelength [[Fig. 8\(a\)](#)]. For uniform pressure application, a stamp would need to conform to such a topography. Meanwhile, typical NIL-produced features, e.g., for photonic devices, will range up to ~ 200 nm, and a reasonable upper limit on the amount of feature distortion would be 5% of the feature size. In [Fig. 8\(a\)](#), these performance limits are bounded by shaded regions on a log-log plot of out-of-plane displacement against in-plane length-scale.

Also plotted are the outputs of [Eq. \(8\)](#), modeling distortions of a hypothetical monolithic stamp with Young's modulus of 100 MPa and Poisson's ratio 0.27, loaded at 100 kPa. The maximum achievable conformation to a sinusoidal surface under these conditions is shown as the solid green line, and the peak distortions of a stamp patterned with a square array of cylindrical protrusions [as defined in [Fig. 2\(c\)](#)] are shown with a dashed green line. Because these modeled deformations lie comfortably between the limits imposed by the wafer topography and acceptable stamp distortions, it is reasonable to suppose that this hypothetical stamp would meet the performance requirements. Young's modulus of 100 MPa is within the range of typical polyurethane stamp materials.

The second example we consider is more challenging. We consider imprinting onto an array of parallel cylinders with radius $50\ \mu\text{m}$ and pitch $100\ \mu\text{m}$, intended to represent the surface of a woven fabric. One might wish to imprint nanostructures onto fibers of a fabric, for example, to impart liquid-repellant properties to it. It would be important for the stamp to contact as much of the fibers' surface area as possible during imprinting. The power spectral magnitude of the simulated surface is found, by Fourier transforming, to be approximately proportional to the 1.6th power of the lateral length scale [[Fig. 8\(b\)](#)]. We again set a constraint of at most

FIG. 8. Examples of tailoring a stamp design to particular substrate topographies. A monolithic stamp is predicted to be acceptable for imprinting onto nominally flat silicon wafers [(a) and (c)]. Measured nanotopographies of three example wafers are shown.⁵¹ A: double-side polished, 350 μm thick; B: double-side polished, 500 μm thick; C: single-side polished, 525 μm thick. Imprinting nano-scale features onto an array of microfibers [(b) and (d)] requires a rigid coating on a compliant base [cross-section shown in (e)] to offer conformation while limiting stamp protrusion distortion. The hypothetical stamps are predicted to conform reasonably well to particle defects [(c) and (d)]: green lines indicate simulated r_k values at $p_0 = 100$ kPa; black dashed lines indicate the limit $r_k = r_0$.

5% distortion of the imprinted features up to a feature size of 200 nm.

The figure shows that in order for a stamp to conform to the fibers while not distorting too much at the feature scale, it needs to have at least two layers: no line with a slope of 1 on the log-log plot of Fig. 8(b) can navigate between the conformation and distortion constraints, and any monolithic stamp has a slope of 1. Instead, we show the model [Eq. (8)] outputs for a stamp with a 50 nm coating of $E_1 = 10$ MPa, $\nu_1 = 0.37$ on a base of $E_2 = 100$ kPa, $\nu_2 = 0.5$, loaded at 100 kPa. This stamp design is predicted to offer the requisite rigidity at sub-micrometer feature sizes while mostly conforming to the micron-scale topography of the fibers. (At $\lambda < 300$ nm, the conformation criterion is still not completely met with this solution, so we would expect some RLT variability in the final imprinted pattern.) Such a stamp could conceivably be made by plasma-oxidizing a 50 nm layer on the surface of a soft silicone elastomer or polymeric gel, or by chemical vapor deposition of a distinct polymeric layer, such as a fluoropolymer, which could also serve as a stamp release layer.

As well as conformation and distortion, the impact of particle defects is checked. The outputs of Eq. (11) are shown in Figs. 8(c) and 8(d) for the two application examples. These results predict that the “kill radius” would be approximately

10 times the particle radius in the first example and only a little more than the particle radius in the second case. While these are simple examples, they illustrate how the dimensionless deformation models of this work can be used to evaluate candidate stamp designs rapidly and identify processing pressures that are likely to be acceptable. Furthermore, these examples suggest a possible general approach to designing a stamp, which is outlined in Sec. S6 in the [supplementary material](#).

V. CONCLUSIONS AND OUTLOOK

We have introduced a computationally inexpensive framework for simulating the elastic deformations of two-material stamps when conforming to complex topographies and particle defects. The use of pre-computed unit-load response functions enables the modeled lateral dimensions to be many orders of magnitude larger than the layer thicknesses without undue computational burden. We have used this framework to establish dimensionless models for (1) the conformation of stamps to sinusoidal topographies, (2) the distortions of the stamp material during printing of specific patterns, and (3) the conformation of stamps to particle defects. These models provide a rapid way to select appropriate stamp elastic properties, layer thicknesses, and loading

conditions for particular nanoimprint or contact-printing processes. Our specific findings are as follows:

- The maximum amplitude of a sinusoidal topography with wavelength λ_s to which a stamp can conform under given loading conditions depends strongly on the ratio of surface layer thickness to wavelength, t_1/λ_s . For $t_1/\lambda_s \leq 4$, conformability is simply proportional to λ_s . For $t_1/\lambda_s \geq 4$, behavior depends on the elastic modulus ratio of the surface/coating (1) and supporting (2) layers. For $E_1 \gg E_2$, the coating layer behaves as a plate on an elastic foundation and deforms by bending, such that conformability scales as λ_s^4 . For $E_1 \ll E_2$, behavior is highly sensitive to how compressible layer 1 is. For reasonably compressible, compliant surface coatings, conformability simply reaches a plateau. As layer 1 approaches incompressibility, however (i.e., $\nu_1 \rightarrow 0.5$), squeeze-film effects within layer 1 become relevant so that conformability actually scales as λ_s^{-2} (i.e., larger wavelengths are more difficult to conform to). For intermediate E_1/E_2 ratios, hybrid behavior is seen.
- The distortion of stamp material around protrusions with particular shapes and with a spatial period of λ_f shows the same essential trends as conformation to sinusoidal topographies. The magnitude of stamp distortions under a given load is also a strong function of the shape of the protrusions. Two examples (parallel ridges and arrayed cylindrical protrusions) are shown in this work although other geometries can be readily simulated with the algorithm presented.
- The ability of a stamp to conform to isolated spherical dust particles with a limited loss of stamp-substrate contact area also depends heavily on the ratio E_1/E_2 . Where $E_1 > E_2$, bulk deformations of the two layers and plate-like bending of layer 1 can both play a role. Where the dust particle radius $r_0 \ll t_1$, local deformations of layer 1 dominate; where $r_0 \sim t_1$, bending of layer 1 plays a major role; and where $r_0 \gg t_1$, layer 1 becomes less relevant and bulk deformation of layer 2 takes over.
- For dust particle conformation with $E_1 < E_2$, on the other hand, we see an unexpected and useful phenomenon whereby the material in the finite-thickness layer 1 can be forced into the gap around the particle, limiting the loss of contact area caused by the dust more effectively than if the entire stamp were made of the more compliant E_1 material. Optimal design conditions of those studied were found to be $t_1 = 2r_0$, $E_2 = 100 E_1$, and $\nu_1 \rightarrow 0.5$. Under these conditions, the uncontacted region can be limited to a target size by applying a load that is just 20% of the load needed for the same performance with a monolithic stamp. Limiting required loads can help to reduce stamp or substrate damage.

The models presented here offer useful guidelines for the design of stamps. It must be borne in mind, however, that a given application can have conflicting requirements which may make it difficult to find a single stamp design that is simultaneously optimal for substrate conformation, pattern distortion control, and particle defect accommodation.

Moreover, particle defects can in practice vary greatly in size, meaning that it may be difficult to select an ideal layer 1 thickness.

Additional factors that are not currently considered in the model, but which may constrain the selection of stamp materials, include differential thermal expansion between the materials in a stamp,⁴⁶ which could lead to unwanted stamp curvature, or between the stamp and the substrate, which may lead to feature smearing and poor layer-to-layer registration. A comprehensive evaluation of a stamp design would not only consider elastic behavior but would confirm whether plasticity and fracture can be avoided during use. In the model presented, stamp protrusions are considered shallow, but in some applications feature buckling and collapse will also be relevant.¹⁴ Finally, because we model stamp layer 2 as a half-space, we do not capture effects where the lateral length-scale of the printed pattern exceeds the true thickness of layer 2. Future models could valuably seek to model the finite thickness of layer 2 and the material that lies behind it. With a full awareness of the assumptions made, however, the present framework can be applied to accelerate and enhance a stamp design.

SUPPLEMENTARY MATERIAL

The online [supplementary material](#) contains additional details of the implementation of the load response functions, finite-element validation of the response functions, the simulation algorithms, simulated shapes of deformed cavity rooves, simulated conformation to spherical particles, and a suggested procedure for designing multilayered stamps.

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