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2016

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Interface bond relaxation on the thermal conductivity of Si/Ge core-shell nanowires

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The thermal conductivity of Si/Ge core-shell nanowires (CSNWs) is investigated on the basis of atomic-bond-relaxation consideration and continuum mechanics. An analytical model is developed to clarify the interface bond relaxation of Si/Ge CSNWs. It is found that the thermal conductivity of Si core can be modulated through covering with Ge epitaxial layers. The change of thermal conductivity in Si/Ge CSNWs should be attributed to the surface relaxation and interface mismatch between inner Si nanowire and outer Ge epitaxial layer. Our results are in well agreement with the experimental measurements and simulations, suggesting that the presented method provides a fundamental insight of the thermal conductivity of CSNWs from the atomistic origin. © *2016 Author(s). All article content, except where otherwise noted, is licensed under a Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by/4.0/).* [http://dx.doi.org/10.1063/1.4940768]

I. INTRODUCTION

Si/Ge core-shell nanowires (CSNWs) have attracted considerable interest for their promising applications in thermoelectric and optoelectronic nanodevices.[1–6] In order to enhance the reliability of these devices, it is paramount to understand the interface effect and relevant thermal transport properties of Si/Ge CSNWs. In comparison to the individual silicon nanowires, Si/Ge CSNWs have evident advantages because the covering layer offers the possibility of a partial and internal charge separation, an efficient passivation of the surface trap states and so on.[7] Up to date, significant progresses for Si/Ge CSNWs both experimentally[8–14] and theoretically[15–28] have demonstrated that the thermal transport properties of Si/Ge CSNWs can be modified at room temperature compared to that of the bare Si or Ge nanowires. Classically, the standard macroscopic approach describing heat transport in semiconductors is the well-known Fourier's law, i.e., $J = -\kappa \nabla T$, where J and ∇T are the heat flux density in the material and the temperature gradient, respectively. However, the validity of $J = -\kappa \nabla T$ is not longer applicable for the nanoscale regime. So this triggered a lot of theoretical works to explore the thermal conductivity of nanostructures.[15–19,24–28]

In fact, as the dimension of a device is reduced to nanometer scale, the effects of surface and interface play an important role in their physical and chemical properties.[29] According to the key idea of atomic-bond-relaxation consideration,[30–34] the bond identities of atoms located at the end parts such as surface and interface will be changed compared to those of the bulk case. Although many efforts about the thermal transport properties of CSNWs have been made to understand the relationship between interface and thermal conductivity, there are many important and fundamental issues remain unsolved. For example, there is a few theoretical investigations account for the coupling role from size and shell effects on thermal conductivity of CSNWs. In particular, the physical origin with regard to interface modulation of CSNWs from viewpoint of atomistic origin is still unclear. Thus, to gain an analytical

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relationship between interface effect and thermal conductivity, more importantly, how to control the thermal transport property in Si/Ge CSNWs, in this contribution we present a theoretical method to clarify the thermal conductivity of Si/Ge CSNWs based on the atomic-bond-relaxation method and continuum mechanics.

II. PRINCIPLE

The schematic illustration of a [110]-oriented Si/Ge CSNW is shown in Fig. 1(a). Note that the Si/Ge CSNW in our case is assumed to be infinitely long (i.e. the length is much greater than the diameter), then we can ignore the effects from both ends. When an epitaxial layer is grown around a bare nanowire, the interface strain will take place due to lattice misfit and can be obtained as $\varepsilon_m = (a_s - a_c^*)/a_c^*$, where a_c^* and a_s are the lattice constants of core interior and that of shell outside.[33,35] Notably, according to atomic-bond-relaxation consideration,[30–34] some quantities, such as lattice constant (a_c^*), bond length (h_0^{c*}) and single bond energy (E_b^{c*}) of the core Si nanowire are different from those of the bulk counterpart.

(a)

(b)

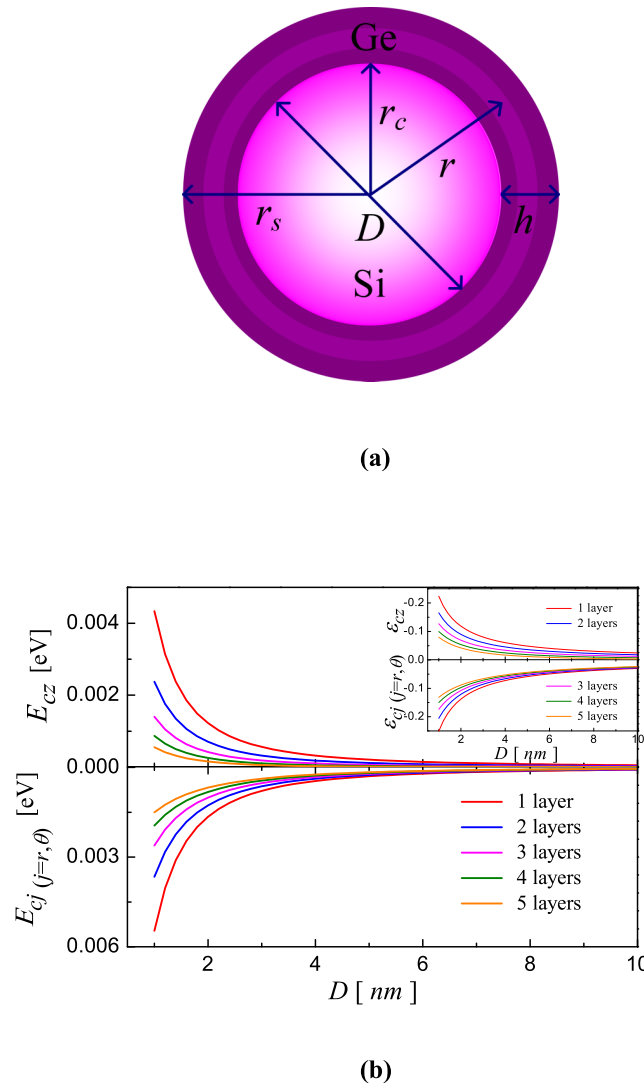FIG. 1. (a) The schematic illustration of a Si/Ge CSNW with core radius r_c, diameter D, shell of radius r_s, local radius of any shell layer r, and shell thickness h. (b) Diameter-dependent elastic energy stored in core Si nanowires under different number of Ge epitaxial layers. The inset in (b) is the diameter dependence of lattice strain in core Si nanowires under different number of Ge epitaxial layers.

In the light of continuum mechanics,[33,35,36] the mean strain and stress in the core nanowire of a CSNW under cylindrical coordinates can be deduced as

$$\langle \varepsilon_{core} \rangle = \begin{cases} -\varepsilon_m (r_s^2 - r_c^2)[f(1-2\nu)+d] & r \text{ or } \theta \text{ direction} \\ \varepsilon_m (r_s^2 - r_c^2) \dfrac{d}{\nu} & z \text{ direction} \end{cases} \tag{1}$$

$$\langle \sigma_j \rangle = \frac{Y \langle \varepsilon_j \rangle}{1-\nu} \ (j=r,\theta,z) \tag{2}$$

where $f = \frac{\nu+1}{(1-k)(1-2\nu)r_c^2 - (1-2\nu+k)r_s^2}$, $d = \frac{\nu}{(r_s^2 - r_c^2)+kr_c^2}$ and $k = Y_c/Y_s$, Y and ν are the Young's modulus and the Poisson's ratio, $\nu = (\nu_c + \nu_s)/2$ is the mean Poisson's ratio, respectively. In contrast to the bulk counterpart, the mean strain existed in the core interior or shell becomes

$$\langle \varepsilon_{\lambda j} \rangle^* = \frac{h_0^{\lambda *}}{h_0^{\lambda}} (\langle \varepsilon_{\lambda j} \rangle + 1) - 1 \tag{3}$$

where the subscript λ, respectively, denotes the core interior and the shell part. h_0^{λ} is the bond length of the bulk.

Theoretically, the cohesive energy of a solid is defined as the energy required to breaking the atoms of the solid into isolated atomic species, which accounts for the binding strength of the crystal. It should be noted that the strain in a material will lead to the atomic bond energy variation. In CSNWs, the single bond energies in the core and the shell will be perturbed by the interface lattice misfit. In reality, the external shell plays an important role in the thermal conduction not only because it can isolate the inner core from the surrounding medium, but also it effectively modulates the strain of these materials and further triggers their elastic energy. Thus the elastic energy can be given by $E_{\lambda j} = S_\lambda h_0^\lambda Y_\lambda \langle \varepsilon_{\lambda j} \rangle^* |\langle \varepsilon_{\lambda j} \rangle^*| /2(1-\nu)$, where S_λ is the cross section area of an atom.

Furthermore, taking the deviation between surface shell and core interior into account, the cohesive energy of the core or shell nanowires can be given by

$$E_{\lambda=c,s}(D) = \sum_{i \leqslant n_s} \left[N_{\lambda i} z_{\lambda i} E_i^{\lambda s} + N_{int} x E_{c-s} + (N_\lambda - N_{\lambda i} - N_{int}\frac{x}{z_{b\lambda}}) z_{b\lambda} E_b^\lambda \right] + \sum_{j=r,\theta,z} N_\lambda z_{\lambda j} E_{\lambda j} \tag{4}$$

where x is the interface composition (the molar ratio). Thus, the relative change of cohesive energy can be obtained

$$\frac{\Delta E_\lambda(D)}{E_\lambda(\infty)} = \sum_{i \leq n_s} \left[\tau_{\lambda i} \left(z_{\lambda i,b} c_{\lambda i}^{-m} - 1 \right) \right] + \tau_{int} \frac{x}{z_{b\lambda}} \left(\frac{E_{c-s}}{E_b^\lambda} - 1 \right) + \sum_{j=r,\theta,z} \left(\tau_{\lambda j} z_{j\lambda,b} \frac{E_{\lambda j}}{E_b^\lambda} \right) \tag{5}$$

where $z_{i\lambda,b} = z_{i\lambda}/z_b$, $z_{j\lambda,b} = z_{j\lambda}/z_b$, E_b^λ and E_{c-s} are the single bond energy in bulk and the interface bond formation enthalpy, $\tau_{i\lambda}$ and τ_{int} are the surface/interface-to-volume ratio, $z_{i\lambda} z_{j\lambda}$ and z_b represent the coordination numbers (CNs) of an atom in the surface and core bulk, $c_i = 2/(1 + \exp((12 - z_i)/8z_i))$ and $\tau_i = \sum_{i < n_s} 4c_i h_0^c/(D+h)$ are the CN-dependent bond contraction coefficient and the surface-to-volume ratio (SVR), respectively.

Aim at clarifying the underlying mechanism on interface and thermal conductivity of CSNWs, the kinetic formula should be taken into account,[37] i.e., $\kappa = \frac{1}{3} cvl$, where v and l are the average phonon velocity and mean free path (MFP), $c = 9Nk_B(\frac{T}{\Theta_D})^3 \int_0^{\Theta_D/T} \frac{y^4 e^y}{(e^y-1)^2} dy$ is the heat capacity of phonons, N, k_B and T denote the number of atoms, Boltzmann constant and temperature, Θ_D is the Debye temperature and $y = \Theta_D/k_B T$. Notably, it was derived for bulk materials. For the mesoscopic system, both the classical approach and the quantum approach encountered some difficulties. Some physical quantities such as heat capacity of phonons, average phonon velocity and MFP remain no longer constants as in the case of bulk material but change with the systems size and interface condition.

Therefore, on the basis of the heat capacity theory and Lindemann's criterion,[38,39] the average phonon velocity can be related with the Debye temperature, so that

$$\frac{v\,(D)}{v\,(\infty)} = \frac{\Theta_D(D)}{\Theta_D(\infty)} = \left[\frac{E_\lambda(D)}{E_\lambda(\infty)}\right]^{1/2} \tag{6}$$

In the case of nanowires, the effective MFP (l_{eff}) should be considered when the length of nanowire (L_z) is not significantly longer than the phonon MFP, i.e., $l_\infty = 20aT_m/(\gamma^2 T)$,[40] where γ is the Gruneisen constant.[41] Thus, we have

$$\frac{1}{l_{eff}} = \frac{1}{l_\infty} + \frac{2}{L_z} \tag{7}$$

As a result, considering the thermal conductivity of a CSNW with rough surface, the surface roughness factor R_f and the exponential suppression $\exp(-l_\infty/D)$ should not be ignored which is incorporated to correct the expressions of $\kappa(D,T)$.[34,37,40] Therefore, in terms of considerations mentioned above, the size- and temperature dependent thermal conductivity of core nanowire can be deduced as follows

$$\frac{\kappa(D,T)}{\kappa_b} = R_f \exp(-\frac{l_\infty^c}{D_c})\left(\frac{T}{T_0}\right)^3 \frac{E_c\,(\infty)}{E_c\,(D)} \frac{l_\infty^c L_z}{l_b^c(L_z + 2l_\infty^c)} \int_0^{\Theta_c(D_c)/T} \frac{y^4 e^y}{(e^y - 1)^2}dy \Big/ \int_0^{\Theta_c(\infty)/T_0} \frac{y^4 e^y}{(e^y - 1)^2}dy \tag{8}$$

In particular, for an infinite system $L_z \sim \infty$, the size dependent thermal conductivity of the core nanowire with smooth surface ($R_f = 1$) under coated epitaxial layers at ambient temperature can be taken as

$$\frac{\kappa(D)}{\kappa_b} = \exp(-\frac{l_b^c E_c(D)/E_c(\infty)}{D}) \int_0^{\Theta_c(D)/T_0} \frac{y^4 e^y}{(e^y - 1)^2}dy \Big/ \int_0^{\Theta_c(\infty)/T_0} \frac{y^4 e^y}{(e^y - 1)^2}dy \tag{9}$$

III. RESULTS AND DISCUSSION

Generally, a bare NW is compressed in the self-equilibrium state due to a large fraction of under-coordinated atoms located at surface. However, in the case of CSNWs, a new self-equilibrium state will start to take place as comparable to that of bare nanowire.[33] Using Eq.(3), we first calculate the size-dependent mean strain existed in the core nanowire, as shown in the inset of Fig. 1(b). The parameters we used in our calculation are listed in Table I. Clearly, the mean compressed strain decreases with increasing shell thickness. Also, the mean strain is decreasing gradually to zero with increasing core diameter and when the CSNWs are very small, the core Si nanowire is compressed by the shell outside due to the discrepancy of lattice constants. Consequently, the strain existing in the core-shell structure will influence the potential field and further disturb the Hamiltonian. From Fig. 1(b), we can clear see that the elastic energy stored in core Si nanowire changes with different number of epitaxial layers. Evidently, the elastic energies of three directions demonstrate an obvious red-shift as the core size are increased to 10 nm, which imply that the external shell can importantly affect the bond identities of the core Si nanowire.

Fig. 2 displays the size-dependent cohesive energy of Si core under different number of Ge epitaxial layers. It is demonstrated that the cohesive energy of core-shell nanostructures is larger than that of the bare nanowires. The reason can be ascribe to the single bond energies in the core and the shell will be perturbed by the interface lattice misfit and surface relaxation.

In order to understand the physical mechanism on thermal conductivity depression of CSNWs, we concentrate on the effects originate from shell thickness and nanowire diameter. As depicted

TABLE I. Calculating parameters of Si and Ge.

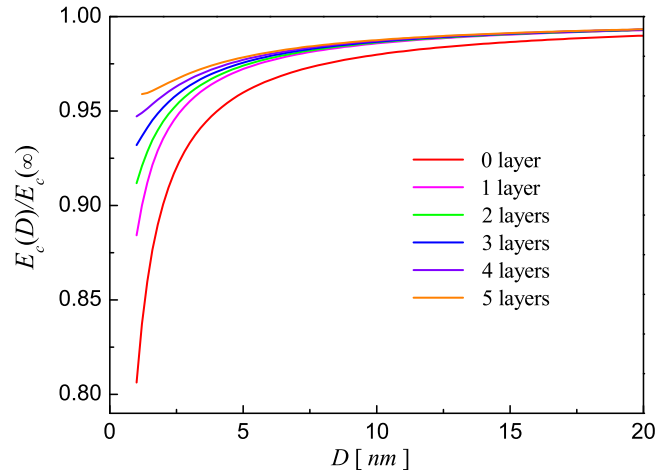|	a_{bulk} (Å)	d_{bulk} (nm)	Θ_D (K)	ν	Y_{110} (GPa)	E_b (eV)	l_b (nm)
Si	5.43[a]	0.235[b]	645[b]	0.218[a]	169.2[a]	0.283[b]	43[b]
Ge	5.65[a]	0.245[b]	374[b]	0.200[a]	137.0[a]	0.228[b]	33[b]

[a]35.
[b]42.

FIG. 2. Diameter-dependent cohesive energy of core Si nanowires under different Ge epitaxial layers.

in Fig. 3(a), the thermal conductivity of Si core decreases significantly with increasing shell thickness. As expected, this trend is very well consistent with the results reported by Hu *et al.*[21] Also, they indicated that the minimum of the overall thermal conductivity of the entire CSNW will be appearance due to larger contribution of coating layer to the overall heat transfer. Fig. 3(b) shows the diameter-dependent thermal conductivity of Si core. Clearly, the thermal conductivity depresses as the diameter decreases, implying that the surface scattering becomes enhancement due to restrained size. Noticeably, our theoretical predictions with corresponding $R_f = 0.4$ are in good agreement with the experimental measurements and simulations.[4,5,37,40] Also, the lower R_f corresponds to the larger surface roughness, which leads to the smaller κ at a fixed diameter, which provides a possible method to modify the thermal conductivity of SiNWs by system size and surface structure. Further, it is found that the thermal conductivity of bare nanowires has the highest value among that of different number of Ge epitaxial layers at a fixed size.

Finally, aim at exploring the interface effect on material's performances, we investigate the thermal conductivity of Si/Ge CSNWs for the case of totally specular scattering, i.e., $R_f = 1$. Notably, the mean strain occurrence in the shell part can be expressed as follows[35]

$$\langle \varepsilon_{shell} \rangle = \begin{cases} \varepsilon_m k r_c^2 [f(1-2\nu) + d - 2f r_s^2 \ln(\frac{r_s}{r_c})/(r_s^2 - r_c^2)] & r \text{ direction} \\ \varepsilon_m k r_c^2 [f(1-2\nu) + d + 2f r_s^2 \ln(\frac{r_s}{r_c})/(r_s^2 - r_c^2)] & \theta \text{ direction} \\ -\varepsilon_m k r_c^2 \dfrac{d}{\nu} & z \text{ direction} \end{cases} \quad (10)$$

Therefore, the overall thermal conductivity of Si/Ge CSNWs in infinite length with overall volume V can be calculated as

$$\frac{\kappa(D)}{\kappa_b} = \sum_{\lambda=c,s} \exp\left(-\frac{l_\infty^\lambda E_\lambda(D)/E_\lambda(\infty)}{D_\lambda}\right) \left(\frac{V_\lambda}{V}\right) \int_0^{\Theta_\lambda(D_\lambda)/T_0} \frac{y^4 e^y}{(e^y-1)^2} dy / \int_0^{\Theta_\lambda(\infty)/T_0} \frac{y^4 e^y}{(e^y-1)^2} dy \quad (11)$$

As illustrated in Figure 4, the effective thermal conductivity of the Si/Ge CSNWs can be shown as a function of the radius ratio for various values of core diameter, in accordance with the available evidences.[15,17,18] It is expected that the thermal conductivity of Si/Ge CSNWs becomes far less as the shell thickness increases. Physically, the increasing of shell thickness has two opposite effects on the thermal conductivity of CSNWs. On the one hand, the effective thermal conductivity changes not only with the composition of the constituents but also with the diameters of the nanowires due to the nature of ballistic phonon transport. On the other hand, this can be explained by considering that the SVR decreases with wire thickness, thus, the interfacial area affected by the Ge epitaxial layers is relatively smaller in thicker wires, leading to higher thermal conductivity for the Si core. Therefore,
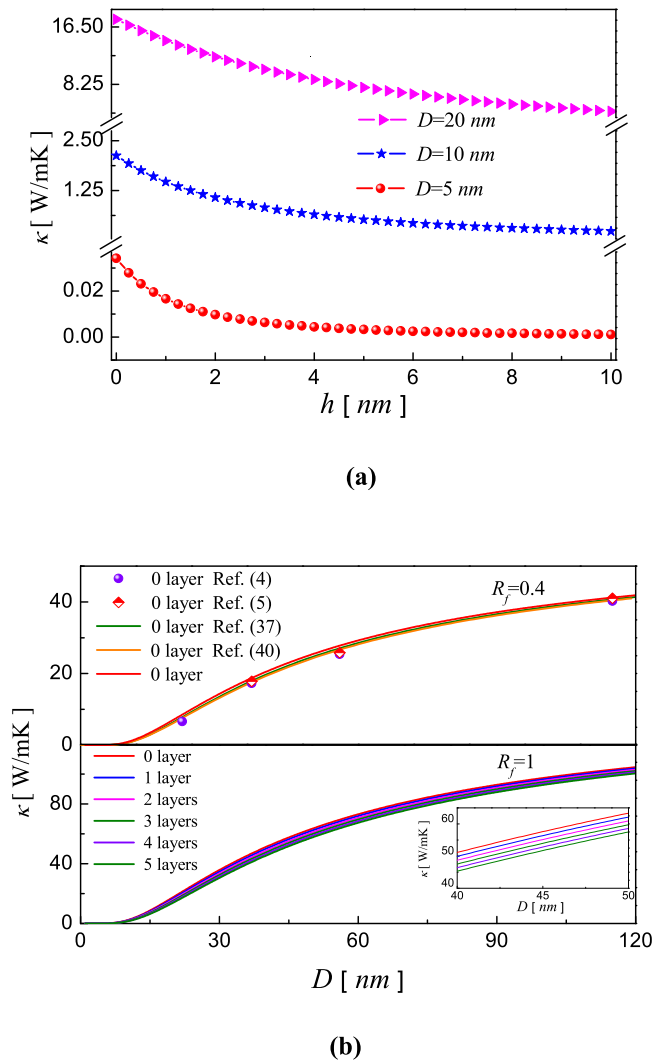
(a)

(b)

FIG. 3. Dependence of the thermal conductivity of Si core on the shell thickness (a) and core diameter (b). The inset in (b) is the magnified area.
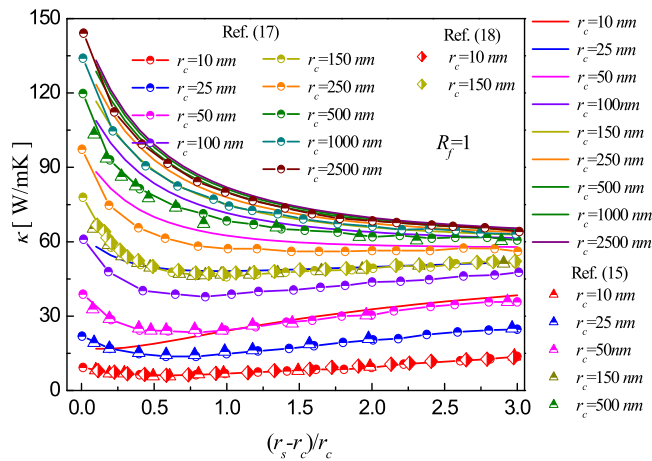

FIG. 4. Thermal conductivities of Si/Ge CSNWs as a function of the radius ratio for the case of totally specular scattering and various radii of core size. The available evidences from Refs. 15, 17, and 18 are represented for comparison.

the results clearly show that the interface scattering plays a crucial role for the thermal conductivity of CSNWs, which leading to the thermal conductivity significant reduction. The underlying mechanism can be ascribed to the lattice strain induced by the CNs deficiencies of surface and interface atoms, which alters the cohesive energy and the thermal conductivity.

IV. CONCLUSION

In summary, based on the atomic-bond-relaxation method and continuum mechanics, we have established an analytic model to pursue the physical mechanism with regard to the interface effect on thermal conductivity of Si/Ge CSNWs. Theoretical results show that the lattice strain existing in Si/Ge CSNWs and associated with elastic energy affect the cohesive energy and thermal transport properties. We have also proposed the relationship between the size and the thermal conductivity and find that the interface in CSNWs can effectively modulate the thermal transport properties. Our predictions are in agreement with theoretical results and experimental observations, which suggest a useful guidance to theoretically design and experimentally control the epitaxial growth of the radial Si/Ge CSNWs for practice applications.

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