<table>
<thead>
<tr>
<th><strong>Title</strong></th>
<th>Calculation of quantum tunneling for a spatially extended defect: the dislocation kink in copper has a low effective mass (Published version)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Author(s)</strong></td>
<td>Vegge, Tejs; Sethna, James. P.; Cheong, Siew Ann; Jacobsen, K. W.; Myers, Christopher R.; Ralph, Daniel C.</td>
</tr>
<tr>
<td><strong>Date</strong></td>
<td>2001</td>
</tr>
<tr>
<td><strong>URL</strong></td>
<td><a href="http://hdl.handle.net/10220/4592">http://hdl.handle.net/10220/4592</a></td>
</tr>
</tbody>
</table>
Calculation of Quantum Tunneling for a Spatially Extended Defect: The Dislocation Kink in Copper Has a Low Effective Mass

Tejs Vegge,1,2 James P. Sethna,3 Siew-Ann Cheong,3 K. W. Jacobsen,1 Christopher R. Myers,4 and Daniel C. Ralph3
1Center for Atomic Scale Materials Physics (CAMP) and Department of Physics, Building 307, Technical University of Denmark, DK-2800, Kongens Lyngby, Denmark
2Materials Research Department, Risø National Laboratory, DK-4000 Roskilde, Denmark
3Laboratory of Atomic and Solid State Physics (LASSP), Clark Hall, Cornell University, Ithaca, New York 14853-2501
4Cornell Theory Center, Cornell University, Ithaca, New York 14853
(Received 9 March 2000)

Several experiments indicate that there are atomic tunneling defects in plastically deformed metals. How this is possible has not been clear, given the large mass of the metal atoms. Using a classical molecular-dynamics calculation, we determine the structures, energy barriers, effective masses, and quantum tunneling rates for dislocation kinks and jogs in copper screw dislocations. We find that jogs are unlikely to tunnel, but the kinks should have large quantum fluctuations. The kink motion involves hundreds of atoms each shifting a tiny amount, leading to a small effective mass and tunneling barrier.

Tunneling of atoms is unusual. At the root, the reason atoms do not tunnel is that their tunneling barriers and distances are set by the much lighter electrons. The tunneling of a proton over a barrier one Rydberg high and one Bohr radius wide is suppressed by the exponential decrease in its effective mass [6]. Because our important conclusions rest upon this delocalization they are qualitatively much less sensitive to the accuracy of our potential calculations for spatially localized tunneling defects. We assert that kinks are likely the only candidate for quantum tunneling in pure fcc metals.

The kink simulation consists of two screw dislocations with opposite Burgers vectors \( \mathbf{b} = \pm \frac{a}{2}[110] \), allowing periodic boundary conditions giving us the perfect translational invariance necessary to measure energy differences to the accuracy we need. The two dislocations are placed in different (111) planes separated by 20 (111) planes (4.4 nm); see Fig. 1. The system is 86 planes wide (19.3 nm) in the two (nonorthogonal) directions, and extends 44.5b (11.4 nm) along the dislocations. We introduce kinks or jogs on the dislocations by applying skew periodic boundary conditions to the system, i.e., we introduce a small mismatch at the interface to the next cell. The procedure also introduces a row of interstitial atoms between the kinked dislocations, which is subsequently removed from the system, leaving us with a total of 329 102 atoms. The kinks have a net line vector of \( \xi_{\text{kink}} = \frac{a}{4}[1T12] \), with \( a \) the lattice constant.

To show how unusual the properties of the kink are, we also study the properties of a dislocation jog. The jog simulation, and the associated energy barrier calculation, is similar and is described elsewhere [7]. The elementary jog we study is introduced with a line vector oriented in the (111) glide plane of the screw dislocation, \( \xi_{\text{jog}} = \frac{a}{4}[1T2] \), which then transforms into an obtuse lower energy configuration: \( \frac{a}{4}[1T2] \rightarrow \frac{a}{4}[1T10] + \frac{a}{4}[011] \). This jog is expected to be the most mobile of the jogs, second only to the kink in mobility.

We introduce the two kinked dislocations directly as Shockley partial dislocations; see Fig. 1, and relax using the MDmin algorithm [8], using effective medium theory: a many-body classical potential [9], which is computationally almost as fast as a pair potential, while still describing the elastic properties well. The elastic constants of...
is the effective mass of the defect incorporating the kinetic energy of the surrounding atoms as they respond adaptively to its motion. The effective mass approximation is usually excellent for atomic tunneling. The method is variational, so Eqs. (1) and (2) remain upper bounds using other assumptions about the tunneling path \( q_i(Q) \) (such as the straight-line path between the two minima described below for the kinks).

The difficulty of finding models for atomic tunneling is illustrated rather well by the properties of the jog we study. The barrier for migration was determined to be 15 meV [7]: lower than other jogs, or even than surface diffusion barriers calculated with the same potential. The effective mass for the jog, estimated by summing the squared displacement of the 200 atoms with largest momentum as the jog moves, is \( M_{\text{eff}}^* \approx 0.36 \) \( M_{\text{Cu}} \). The jog is spatially localized (it does not dissociate into partials), with a few atoms in the core of the jog carrying most of the motion. The WKB tunneling matrix element for the jog to tunnel a distance \( Q = 2.5 \) Å over a barrier \( V = 0.015 \) eV is suppressed by a factor of roughly \( \exp(-\sqrt{2M_{\text{eff}}^* V / \hbar}) \approx 10^{-14} \). Jogs do not tunnel much.

For the kinks, we take a relaxed initial configuration and define a final configuration with the kink migrated by one lattice spacing along the dislocation. The final position for each atom is given by the position of the neighboring atom closest to the current position minus the kink migration vector \( \mathbf{\xi}_{\text{migr}} = \frac{a}{2}[110] \) which represents the net motion of the kink. This automatically gives the correct relaxed final position, which is otherwise difficult to locate given the extremely small barriers. The width of the kinks is the traditional name for their extent along the axis of the screw dislocation. We can measure this width by looking

The potential are \( C_{11} = 176.2 \) GPa, \( C_{12} = 116.0 \) GPa, and \( C_{44} = 90.6 \) GPa with a Voigt average shear modulus of \( \mu = 66 \) GPa, and an intrinsic stacking fault energy of \( \gamma_1 = 31 \) ml/m².

We present three quantities for the kink and jog: the Peierls-like barrier for migration along the dislocation, the effective mass, and an upper bound for the WKB factor supressing quantum tunneling through that barrier. Since the motion of these defects involves several atoms moving in a coordinated fashion, we use instantons: the appropriate generalization of WKB analysis to many-dimensional configuration spaces [6,10,11]. An upper bound for the tunneling matrix element is given by the effective mass approximation [11,12],

\[
\Delta \leq \hbar \omega_0 \exp \left( -\int \sqrt{2M^*(Q)V^*(Q) dQ / \hbar} \right),
\]

where \( \omega_0 \) is an attempt frequency, \( V^*(Q) \) is the energy of the defect at position \( Q \) with the neighbors in their relaxed, minimum energy positions \( q_i(Q) \), and

\[
M^*(Q) = \sum_i M_i (d_{qi} / dQ)^2
\]
at the net displacement of atoms between the initial and final configurations. We find that this displacement field is localized on two partial kinks; Fig. 2 shows it along lines through the cores of the partial dislocations described in Fig. 1. These two partial kinks are quite wide (13b and 21b). They differ because the partials are of mixed edge and screw character; it is known [13] that the kink which forces a mixed dislocation towards the screw direction will be wider and have higher energy. This is wider than the \( w \approx 10b \) predicted for slip dislocations in closed-packed materials by Hirth and Lothe, and Seeger and Schiller using line tension models [14]. The kinks will merge together for kink densities above one per kink width, or dislocation line tension models [14]. The kinks will merge together for kink densities above one per kink width, or dislocation radius of curvature smaller than the width squared over \( \pi \) for \( \kappa > 10^3 \), validating the traditional description of continuously curved dislocations.

Notice that the maximum net distance moved by an atom during the kink motion in Fig. 2 is around 0.01 Å. Summing the squares of all the atomic motions, and using Eq. (2), we find an effective mass \( M_{\text{eff}}^k = M_C/130 \) within the straight-line path approximation. This remarkably small mass can be attributed to three factors. (1) The mass is decreased because the screw dislocation is split into two partial dislocations [15]. (2) The cores of the partial dislocations are spread transversally among \( W_T = 4 \) planes of atoms, Fig. 3; this factor seems to have been missed in continuum treatments. These first two factors each reduce the total distance moved by an atom as the kink passes from \( z = -\infty \) to \( +\infty \). (3) The kinks on the partials average \( W_L = 17 \) planes wide (above), so the total atomic motion is spread between around 17 kink migration hops [16]. Thus when the kink moves by \( x \), the atoms in two regions \( 1/W_L \) long and \( 1/W_T \) wide each move by \( x/(2W_LW_T) \), reducing [16] the effective mass by roughly a factor of \( 2W_LW_T \sim 136 \).

Evaluating the energy at equally spaced atomic configurations and linearly interpolating between the initial and final states (along the straight-line path) yields an upper bound to the kink-migration barrier of 0.15 µeV, Fig. 4. We attribute this extremely small barrier to the wide kinks on the partials: for wide kinks the barrier \( V \) should scale exponentially with the ratio of the kink width to the interplanar distance: \( V \propto \exp(-W_L) \) [17].

This small barrier is not only negligible for thermal activation (2 mK), but also for quantum tunneling. The WKB factor suppressing the tunneling would be \( \exp(-\sqrt{2m^*W_LQ}/\hbar) = \exp(-0.0148) = 0.985 \). Even at zero temperature, the kinks effectively act as free particles, as suggested in the literature ([13], among others).

Our estimated kink migration barrier is thus \( 10^5 \) times smaller than that for the most mobile of the jogs. How much can we trust our calculation of this remarkably small barrier? Schottky [18] estimates using a simple line tension model that the barrier would be \( \sim 3 \times 10^{-5} \) eV in fcc materials, using a Peierls stress \( \sigma_P = 10^{-2} \mu \) and a kink width \( w = 10b \). This value is a factor of 200 higher than the barrier we find. On the other hand, both experiments and theoretical estimates predict \( \sigma_P = 5 \times 10^{-6} \mu \) for Cu [17], yielding barriers orders of magnitude lower than ours. Using a classical potential is valid for our purposes: electronic quantum fluctuations are well treated in the Born-Oppenheimer approximation, and atomic quantum fluctuations are explicitly treated in the instanton approximation. The interatomic potentials we use do not take into account directional bonding. This is usually a good approximation for noble metals; however, small contributions from angular forces may change the kink width. The kink width is like an energy barrier, balancing different competing energies against one another: in analogy, we

---

**FIG. 3.** The magnitude of the atomic displacement field as the two partial kinks move, along the cores of the two partial dislocations, as a function of the \( x \) coordinate. The core regions are fitted to two squared Lorentzian distributions. The partial core widths \( W_T = 4d \) [4 (111) lattice planes], significantly reduce the effective mass of the kink.

**FIG. 4.** The activation energy as a function of the straight-line distance moved by the kink on one dislocation, with an associated barrier of \( E_{\text{act}} = 0.15 \mu \) eV. Notice that this activation energy is about one part in \( 10^{13} \) of the total system energy.
expect it to be accurate to within 20% or 30%. Our small value for the effective mass, dependent on the inverse cube of the spatial extent of the kink, is probably correct within a factor of 2. The energy barrier is much more sensitive: if we take the total exponential suppression to be $10^5$ (using the jog as a “zero-length” defect) then each 20% change in the width would yield a factor of 10 change in the barrier height. The qualitative result of our calculation, that the barriers and effective masses are small, is robust not only to the use of an approximate classical potential, but may also apply to other noble metals and perhaps simple and late transition metals.

Quantum creep estimates [3] of double-kink nucleation will change significantly using our low kink effective mass. The glassy low-temperature properties [4] of deformed metals probably arise from kinks tunneling between pinning sites. (Dislocation-rich metals are not glasses, and glasses do not have kinks, but there has been speculation [19] that tunneling in glasses is collective.) We do not have an explicit model for the scaling seen in nanoconstrictions [5], but we do claim that kinks are the only active atomic degrees of freedom.

In summary, we have used an atomistic calculation with classical potentials to extract energy barriers and effective masses for the quantum tunneling of dislocation jogs and kinks in copper. For jogs, the atomic displacements during tunneling are primarily localized to a few atoms near the jog core, each moving a significant fraction of a lattice spacing. Consequently, the tunneling barrier and effective mass are relatively large, and tunneling is unlikely. However, the kinks in screw dislocations are much more extended: as a kink moves by one lattice spacing, hundreds of atoms shift their positions by less than 1% of a lattice spacing. Both the energy barrier and the effective mass are reduced, to the extent that tunneling should occur readily. Kinks are likely the only candidate for quantum tunneling in pure crystalline materials. They may be the source of quantum creep, glassy internal friction, and nonmagnetic Kondo effects seen in plastically deformed metals.

This work was supported by the Digital Material Project NSF No. 9873214, the Danish Research Councils through Grant No. 9501775, and the Center for Structural Characterization and Modelling of Materials in Risø. The Center for Atomic-scale Materials Physics (CAMP) is sponsored by the Danish National Research Foundation. An equipment grant from Intel and the support of the Cornell Theory Center, including through Grant NSF No. EIA-9972853, are also gratefully acknowledged. We had helpful conversations with Nicholas Bailey and Jakob Schiøtz.