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# Comment on "Glide Systems and Peierls Stresses in f.c.c. and b.c.c. Metals From Phonon Energies"

## **Abstract**

The theory of Boffi *et al.* of Peierls stresses in crystals is criticized on physical grounds on a number of points.

## **Keywords**

Phonons

## **Disciplines**

Engineering | Materials Science and Engineering | Metallurgy | Semiconductor and Optical Materials

## **Comments**

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# Comment on "Glide systems and Peierls stresses in fcc and bcc metals from phonon energies"

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(Received 10 December 1973)

The theory of Boffi *et al.* of Peierls stresses in crystals is criticized on physical grounds on a number of points.

Recently, Boffi, Caglioti, Rizzi, and Rossitto<sup>1</sup> presented a calculation of the Peierls stresses in crystals based on the Frenkel-Kontorova model with appropriate constants computed from measured phonon frequencies. Within the framework of the model, calculations in their paper are correct; however, any variation of the Frenkel-Kontorova model suffers two major defects—namely, the model is one dimensional and it applies to the edge dislocation only. For a number of years atomistic models which are three dimensional in concept have been developed<sup>2</sup>; these apply equally well to both edge and screw dislocations and are much more realistic. It seems unlikely that a model so primitive in concept as the Frenkel-Kontorova model is able to give results which can be compared even qualitatively with measured experimental values on real metals; any correlation is almost bound to be fortuitous.

There are a number of specific physical criticisms which can be made regarding both the calculations and interpretations of Boffi *et al.*<sup>1</sup>

(i) The atomic displacements in the dislocation core are relatively very large and well outside the framework of the harmonic approximation. Measured phonon frequencies give information about the interatomic forces for only small deviations of the atoms from their equilibrium positions; therefore, such results cannot be used to calculate the forces between atoms in the dislocation core. It is, of course, the structure of the core which determines the Peierls stress.

(ii) As the authors state, in anisotropic crystals it is not possible to deduce the parameter  $K$  [Eq. (11) of Ref. 1] from phonon-dispersion curves for the (111)  $[10\bar{1}]$  and (101)  $[11\bar{1}]$  slip systems. Since these systems play the major role in the deformation of fcc and bcc crystals, respectively, it is of paramount importance that they should be included in any calculation on plasticity.

(iii) In Table III of Ref. 1, the differences in the Peierls energies and stresses in columns A, B, and C are due to differences in a parameter  $P=K/A$ , where  $K$  and  $A$  are calculated from the phonon-dispersion data, continuum elasticity theory, and a mixture of the two. The values of these parameters for different columns are not given, but they certainly have a profound effect on the Peierls stress which can vary for a particular slip system by more than  $10^4$  times (e.g., Nb (101)  $[010]$ ). When such a massive variation in a calculated value is possible, a model should be capable of accounting for any experimental results, but such sensitivity makes the model most unsatisfactory.

(iv) The Frenkel-Kontorova model most closely resembles an edge dislocation; in bcc materials it is

generally accepted that the Peierls stress measured in plasticity experiments is that of a screw dislocation since screws are thought to be much more difficult to move than edges.<sup>3</sup>

(v) As the authors point out, the only comparison of the numerical value of the Peierls stress between their theory and experiment is for tungsten. Any comparison between calculated Peierls stresses and experimental results should be for experiments near 0°K (in practice liquid-helium temperature, 4.2°K) since at higher temperatures thermal fluctuations help the dislocations to overcome the Peierls barrier, and the applied stress is lowered. However, Boffi *et al.* give a reference to Vreeland<sup>4</sup>; Vreeland's paper did not contain any original work on tungsten but included results of Schadler<sup>5</sup> who measured the velocity-stress dependence of edge dislocations in the microstrain region at 298 and 77°K. There is, however, a much more serious error in Boffi *et al.*; they quote the critical resolved shear stress as  $\approx 20 \times 10^5$  dyn cm<sup>-2</sup>. It appears that they have misread the graph in Ref. 4 since the abscissa is a logarithmic scale. The yield stress at 77°K given by Schadler<sup>5</sup> is  $\approx 5 \times 10^9$  dyn cm<sup>-2</sup> ( $\approx 7 \times 10^4$  psi), although, of course, some dislocations do move with very low velocities at somewhat lower stresses. However, from what we have said above about thermal fluctuations, the Peierls stress will be greater than the yield stress at 77°K perhaps by a factor of  $\sim 2$ . In any case, comparison of the model by Boffi *et al.* with experiment is now very poor; their Peierls stress for tungsten is nearly  $10^5$  times smaller than the yield stress at 77°K, a difference which is unlikely to be explained on the basis of "friction processes". Clearly, the model has failed completely in this instance, even the result for  $P$  calculated from continuum elasticity (column C of Ref. 1) is far superior ( $2.2 \times 10^8$  dyn cm<sup>-2</sup>).

(vi) Boffi *et al.* completely ignore the majority of work on niobium in claiming that the preferred deformation system is (101)  $[010]$ . The  $\langle 111 \rangle$  slip direction is now rarely reported explicitly since it is so well established, but it is determined routinely in slip-line analysis from observation of the "dead band" and/or from rotation of the tensile axis; also electron microscopy shows a preponderance of  $\langle 111 \rangle$  dislocations (see, for example, Refs. 6 and 7, and for a review, Ref. 3). Furthermore, what Reid, Gilbert, and Hahn<sup>8</sup> observed was not a set of slip lines but a deformation zone just prior to (chisel) fracture; the actual measured shear direction was up to 15° away from the  $\langle 100 \rangle$  direction. Mason and MacDonald<sup>9</sup> did not, in fact, determine the glide direction as  $\langle 100 \rangle$ , but rather claim that their results on dislocation damping at frequencies of 10–150

MHz are consistent with dislocations with  $\langle 100 \rangle$  Burgers vectors and quote Reid *et al.* as their reference.

Apart from these detailed criticisms we would like to emphasize again that crude models such as those based on the one-dimensional Frenkel-Kontorova formulation are not likely to contribute to the theory of the dislocation core structure and the Peierls stresses in real metals. This can only be achieved by three-dimensional atomistic models which can reveal the core structure and dislocation behavior unpredictable on the basis of an oversimplified model; an example is the case of the screw dislocation in bcc crystals.<sup>10,11</sup> These calculations require some assumptions about the interatomic forces for large displacements of the atoms from their equilibrium positions. An atomistic three-dimensional method which uses the information about the forces for small displacements of the atoms has also been developed and is known as lattice statics<sup>12</sup>; this method cannot be used to study the dislocation core, but to calculate, for example, displacements outside the core taking into account that the dislocation is in a crystal lattice rather than in an elastic continuum. The information extracted from the phonon-dispersion data can be introduced into lattice statics directly via the lattice Green function.<sup>13,14</sup>

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