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Stress dependence of the Peierls barrier of 1/2⟨1 1 1⟩ screw dislocations in bcc metals

R. Gröger [a,*], V. Vitek [b]

[a] Central European Institute of Technology – Institute of Physics of Materials (CEITEC-IPM), Academy of Sciences of the Czech Republic, Žižkova 22, 61662 Brno, Czech Republic

[b] Department of Materials Science and Engineering, University of Pennsylvania, 3231 Walnut Street, Philadelphia, PA 19104, USA

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Abstract

The recently formulated constrained nudged elastic band method with atomic relaxations (NEB + r) (Gröger R, Vitek V. Model Simul Mater Sci Eng 2012;20:035019) is used to investigate the dependence of the Peierls barrier of 1/2⟨1 1 1⟩ screw dislocations in body-centered cubic metals on non-glide stresses. These are the shear stresses parallel to the slip direction acting in the planes of the ⟨1 1 1⟩ zone different from the slip plane, and the shear stresses perpendicular to the slip direction. Both these shear stresses modify the structure of the dislocation core and thus alter both the Peierls barrier and the related Peierls stress. Understanding of this effect of loading is crucial for the development of mesoscopic models of thermally activated dislocation motion via formation and propagation of pairs of kinks. The Peierls stresses and related choices of the glide planes determined from the Peierls barriers agree with the results of molecular statics calculations (Gröger R, Bailey AG, Vitek V. Acta Mater 2008;56:5401), which demonstrates that the NEB + r method is a reliable tool for determining the variation in the Peierls barrier with the applied stress. However, such calculations are very time consuming, and it is shown here that an approximate approach of determining the stress dependence of the Peierls barrier (proposed in Gröger R, Vitek V. Acta Mater 2008;56:5426) can be used, combined with test calculations employing the NEB + r method.

Keywords: Screw dislocation; Peierls barrier; Nudged elastic band; Bcc metals; Peierls stress

1. Introduction

The most outstanding aspects of the plastic deformation of single crystals of body-centered cubic (bcc) metals are the rapid increase in the flow stress with decreasing temperature and increasing strain rate, a strong dependence of the flow stress on the orientation of the crystal relative to the loading axes, and the related breakdown of the Schmid law (for reviews, see Refs. [4–8]). It has been firmly established in the last forty years that this plastic behavior results from sessile 1/2⟨1 1 1⟩ screw dislocations whose cores spread into three {1 1 0} planes of the ⟨1 1 1⟩ zone. These dislocations then possess a very high Peierls stress, and their motion does not obey the Schmid law (for reviews, see e.g. Refs. [5,9]). At finite temperatures, their movement is aided by thermal activation via nucleation of pairs of kinks that subsequently migrate easily along the dislocation line [10–13].

While many atomistic calculations of the core structure of 1/2⟨1 1 1⟩ screw dislocations in bcc metals, as well as the stress needed to move them at 0 K (the Peierls stress), have been made (for a recent review, see Ref. [9]), studies of their thermally activated motion are much rarer. In principle, atomistic modeling of the dislocation motion via formation and propagation of kink pairs can be made by molecular dynamics, and several such calculations were performed [14–17]. Notwithstanding, owing to the limited timescale of molecular dynamics studies at room or lower temperatures, such calculations had to be carried out at stresses

* Corresponding author.
E-mail address: groger@ipm.cz (R. Gröger).

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and strain rates several orders of magnitude higher than those of interest in the usual deformation experiments. However, such large strain rates may only be encountered in shock loading, but then the deformation process is not controlled by the formation of kink pairs. Instead, other phenomena such as phonon and electron scattering become dominant (see e.g. Refs. [18–21]).

An alternative though more approximate approach is to develop a mesoscopic model based on the reaction rate theory describing the thermally activated process of the formation of pairs of kinks [10–13]. However, when dislocation core effects are involved, such models depend sensitively on the form of the Peierls barrier $V(\xi)$ that the dislocation has to overcome when moving in the crystal along a generally curvilinear coordinate ξ. The reason is that the activation enthalpy, which determines the rate of the dislocation motion, is obtained by integrating over the Peierls barrier, and this integration requires knowledge of the overall shape of this barrier [22–25]. This information is not obtained in the molecular statics calculations, because these reveal only the core structure and the stress at which the dislocation moves at 0 K, i.e., the Peierls stress σ_P. The only information about the Peierls barrier that can be acquired from these calculations is its maximum slope in the direction of the dislocation motion since

$$\sigma_P b = \max(\mathrm{d}V/\mathrm{d}\xi), \tag{1}$$

where V is the energy per unit length of the dislocation, and b is its Burgers vector. At the same time, the dependence of the Peierls stress on the character of the applied load, which is crucial information needed in the analysis of the deformation behavior of bcc metals, is obtained in the molecular statics calculations. This has to be reflected in the corresponding dependence of the Peierls barrier on the type of loading.

In molecular statics calculations that apply a pure shear stress parallel to the Burgers vector of a $1/2\langle 1\,1\,1\rangle$ screw dislocation, the Peierls stress was generally found to depend on the orientation of the maximum resolved shear stress plane (MRSSP) [2,5,26–28]. This dependence is the origin of the so-called twinning–antitwinning asymmetry found in virtually all bcc metals [4]. However, calculations in which the stress tensor corresponds to tension/compression revealed a strong dependence of the Peierls stress on the shear stress applied perpendicular to the Burgers vector [2,26–28]. This stress does not contribute to the Peach–Koehler force on the dislocation, but affects the magnitude of the Peierls stress indirectly by modifying the structure of the dislocation core. Both the effect of the orientation of the MRSSP and the shear stress perpendicular to the Burgers vector imply that the Peierls barrier is not a fixed function determined purely by the material, as often assumed, but is an explicit function of the applied stress tensor. This is one of the major results of molecular statics studies of the structure and motion of $1/2\langle 1\,1\,1\rangle$ screw dislocations in bcc metals published recently [2]. Moreover, this conclusion is most likely general whenever the dislocation core is not planar. For example, an analogous conclusion was reached in the study of the Peierls barrier of the sessile Lommer–Cottrell dislocation [17]. Consequently, knowledge of the dependence of the Peierls barrier on the applied stress tensor is essential for obtaining the appropriate stress dependence of activation enthalpies and thus to develop a mesoscopic model of thermally activated dislocation motion that includes this dependence.

The calculation of the Peierls barrier can be made using the nudged elastic band (NEB) method, originally developed for studies of chemical reactions [29,30]. Within this method, the minimum energy path of the dislocation between two neighboring lattice sites of the same energy is found and the variation in the dislocation energy along this path is identified with the Peierls barrier. Such calculations were made recently using several empirical schemes to describe the interaction between the atoms as well as methods based on the density functional theory (DFT) [1,17,31–34].

The goal of the present study is to investigate the dependence of the Peierls barrier on the applied shear stresses parallel and perpendicular to the slip direction that were found to control the Peierls stress [2,27]. For this purpose the Peierls barrier and its stress dependence were determined using the NEB method with constrained atomic relaxations (NEB + r), which the present authors formulated recently [1]. While the present calculations have been carried out mainly using the bond order potential for tungsten [35], the findings are likely to be more general and apply broadly to all bcc metals.

In these calculations, it is considered that the dislocation may move by elementary steps on three $\{1\,1\,0\}$ planes of the zone of the common $\langle 1\,1\,1\rangle$ slip direction, as revealed by molecular statics calculations of the dislocation motion at 0 K [2,27]. First, the variation in the Peierls barrier is studied when a pure shear stress parallel to the Burgers vector is applied in planes inclined with respect to the $\{1\,1\,0\}$ plane on which the dislocation glide takes place. Next, the Peierls barriers are evaluated for the dislocation motion on the three $\{1\,1\,0\}$ planes of the $[1\,1\,1]$ zone under zero and applied positive and negative shear stresses perpendicular to the slip direction as well as for the combination of shear stresses parallel and perpendicular to the slip direction. The corresponding Peierls stresses determined from the maximum slopes of these barriers are then compared with those found in molecular statics calculations at 0 K. This comparison illustrates the full consistency of the two approaches. In addition, the case of uniaxial loading is also investigated. Finally, the Peierls barriers obtained from the NEB + r calculations are compared with those estimated previously [3] using only knowledge of the Peierls stress, and the limits of the latter approximate but computationally much less demanding approach are assessed.

2. Theoretical and computational background

Within the NEB method [29,30,36,37], the path of a given system is viewed as a chain of states between its