

On the dislocation properties of 60° partial dislocation in silver: core structure and Peierls stress

Shao-Rong Li^a, Shao-Feng Wang^a, Qun-Yi Wei^b, and Xiao-Zhi Wu^{a,*}

^a Institute for Structure and Function, Chongqing University, Chongqing 400044, China

^b College of Materials Science and Engineering, Chongqing University, Chongqing 400044, China

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Abstract. Two-dimensional modified Peierls-Nabarro dislocation equation concerning the discreteness of crystals is reduced to one-dimensional equation to determine the core structure of partial dislocation in Ag. The generalized stacking fault energy along the Burgers vectors of partial dislocation is a skewed sinusoidal force law, which is related to the intrinsic stacking fault energy and the unstable stacking fault energy. A trial solution appropriate for arbitrary dislocation angle is presented within the variational method. The results show that the half core width increases as the increase of dislocation angle. Moreover, the core width decreases with the increase of the unstable stacking fault energy and the intrinsic stacking fault energy. Peierls stress for 60° partial dislocation is in agreement with the experimental results.

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Key words: core structure, partial dislocation, variational method, Peierls stress

1 Introduction

It is widely accepted that extended defects such as dislocations play an important role in defining the mechanical properties of materials [1–5]. In face-centered-cubic (fcc) crystals (such as Ag), the glide dislocations should be dissociated into two Heidenreich-Shockley partial dislocations bounding a stacking fault ribbon among them [6,7]. The dissociation properties make the procedure to determine the mobility of dislocations (Peierls stress) more complex and questionable. Two types of theoretical approaches have been applied to examine the Peierls stress of dissociated dislocations. The first type is based on the direct atomistic simulation using empirical interatomic potentials [8–11]. The second one employs the Peierls stress of single partial dislocation to replace that of the dissociated

*Corresponding author. *Email address:* xiaozhiwu@cqu.edu.cn (X. Z. Wu)

dislocation within the framework of Peierls-Nabarro (P-N) model. The atomistic simulations may not be reliable as the empirical potentials are used. On the other hand, the P-N model provides a conceptual framework for the prediction of the size and mobility of dislocations, namely core structure and Peierls stress [6]. However, a quantitative agreement with experiments has been lacking as the model is essentially a continuum treatment.

Recently, the boundary problem of the half-infinite lattice has been solved by using the lattice Green function method. By virtue of the solution obtained in the boundary problem, a set of dislocation equations have been derived explicitly for the two-dimensional triangular lattice. The dislocation equation only related to displacement of the atoms on the border. Because the displacement field of a dislocation varies slowly in the space, the discrete dislocation equation can be changed into the integro-differential equation, namely the modified P-N dislocation equation [12–14].

In this paper, we focus on the core structure properties and Peierls stress for 60° partial dislocation in Ag. We choose to study 60° partial dislocation in Ag for two reasons: (i) the intrinsic stacking fault energy ($\gamma_I = 0.021 \text{ Jm}^{-2}$) is small and dissociation equilibrium distance is large enough so that two partial dislocation should not overlap too much, (ii) the edge dislocation dissociates into two 60° partial dislocations and the Peierls stress of single partial dislocation used to replace the dissociated dislocation is more reasonable [15]. In Section 2, the core structure properties of partial dislocation are investigated with the modified P-N equation. Peierls stress for 60° partial dislocation in Ag is presented in Section 3. Finally, conclusions are made in Section 4.

2 Core structure of partial dislocations with skewed sinusoidal force law

The 2D modified P-N dislocation equation for straight dislocations that describe the balance of atoms on the border based on the lattice dynamics and the symmetry principle takes the following form [14]

$$-\frac{\beta_e}{2} \frac{d^2 u^x}{dx^2} - \frac{K_e}{2\pi} \int_{-\infty}^{+\infty} \frac{dx'}{x' - x} \left(\frac{du^x}{dx} \right) \Big|_{x=x'} = f^x(u^x, u^y), \quad (1)$$

$$-\frac{\beta_s}{2} \frac{d^2 u^y}{dx^2} - \frac{K_s}{2\pi} \int_{-\infty}^{+\infty} \frac{dx'}{x' - x} \left(\frac{du^y}{dx} \right) \Big|_{x=x'} = f^y(u^x, u^y), \quad (2)$$

where K_e and K_s are the energy factors of the edge and screw dislocations, u^x and u^y are the edge and screw components of displacements. For the isotropic solid, $K_e = \mu\sigma/(1 - \nu)$ and $K_s = \mu\sigma$, with μ being shear modulus and ν Poisson's ratio, σ is the area of the primitive cell of the misfit plane. The coefficients of the second-order derivations β_e and