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Effect of a generalized shape Peierls potential and an external stress field on kink mechanism in a continuum model

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The $a_0/2\langle 111\rangle$ screw dislocation glides through the nucleation and propagation of the kink-pair which dominates the plastic deformation of the BCC iron. A continuum model and the corresponding numerical methods are developed to investigate the kink mechanism on an arbitrary shape Peierls potential and subject to an external stress field. This model gives a link between the Landau theory of phase transitions and the line tension theory of string models. The order parameter is associated with the screw dislocation in BCC iron for describing the relative slip between adjacent Peierls valley. The kink configurations on the different Peierls potentials, such as the sinusoidal, Eshelby, anti-parabolic and camel-hump potential, are derived. By considering the motion of the screw dislocation on a 2-D Peierls potential surface, the 3-D saddle-point configuration of a non-planar kink-pair is obtained. The configuration is directly related to the details of the 2-D potential surface and it changes along with the applied stress tensor. A parameterized constitutive equation is derived for describing the temperature dependence of the flow stress which is compared with the experimental data from literature. The twinning/anti-twinning (T/AT) asymmetry and the tension-compression (T/C) asymmetry are reproduced in the model. The results rule out the possibility that the non-Schmid plasticity of the BCC iron is ascribed to split configuration.

1. Introduction

The plastic anisotropy of the BCC iron can be ascribed to the $a_0/2\langle 111\rangle$ screw dislocation with a non-planar core (Duesbery and Vitek, 1998; Edagawa et al., 1997b). The slip and cross-slip behaviors of the screw dislocation are controlled by the kink mechanism. The stress-temperature relation of kink mechanism is used for explaining the non-Schmid plasticity and temperature-dependent yield stress of the BCC metals (Brunner and Diehl, 1991; Castillo-Rodríguez and Sigle, 2011; Li et al., 2014; Mitchell et al., 1999). The nucleation energy of a kink-pair as a function of local stress is an important case to the molecular-dynamics (MD) of the discrete system (Chaussidon et al., 2006; Khater et al., 2014; Stukowski et al., 2015; Wen and

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Ngan, 2000), here we provide a continuum model for an understanding of the kink mechanism based on a phase field theory by treating the nucleation of kink-pair as a first order phase transition.

The shape of the Peierls potential dominates the configuration and energy of the kink-pair. Several models and theories were developed to study this problem, and they could be classified either the line tension theory or the elastic interaction theory. The line tension theory treats the dislocation line as a string moving on a periodic substrate potential, a number of methods are proposed based on this idea, such as the line tension model (LT) (Dorn and Rajnak, 1964), the line energy model (LE) (Schulze and Vohringer, 2000), the discrete Frenkel-Kontorowa (FK) model and the developed discrete Frenkel-Kontorova-Langevin (FKL) model (Gornostyrev et al., 1999, 2002; Rodney and Proville, 2008; Swinburne et al., 2013). As an example, the excellent review written by Pierre Guyot and John E. Dorn, several issues like the nucleation enthalpy, the activation volume, and the stress-temperature relation of the velocity of the kink-pair were summarized based on a simple line tension model (Guyot and Dorn, 1967). It should be noted that the line tension models in Guyot and Dorn's work and the more pre-existing works all neglected to take into account the periodic force exerted on the dislocation line, that their mechanical equilibrium equation did not include the derivatives of Peierls potential with respect to the dislocation segments' position. Until Hirokazu Koizumi et al. first derived the precise equilibrium equation including this term, which showed as a perturbed sine-Gordon (SG) equation (Koizumi et al., 1994). Then, Keiichi Edagawa et al. extended this model to a three dimensional one for investigating the non-Schmid law in a cross-slip system (Edagawa et al., 1997a). K. Srivastava et al. re-investigated this problem in tungsten and compared the line tension model's results with the data from discrete dislocation dynamics (Srivastava et al., 2013). M. Itakura et al. employed a discrete form of this model for studying the mobility of screw dislocation of body-centered cubic (BCC) iron, several possible migration paths of a screw dislocation between the hard core, split core and easy core position on $\{110\}$ plane were investigated on a 2D Peierls potential surface calculating by the first-principle study (Itakura et al., 2012). A year later, they extended this discrete line tension model to study the interaction between a kink-pair and a hydrogen atom by implanting a Lorentzian function for describing the hydrogen binding energy (Itakura et al., 2013). It needs to be noted, although a discrete form of Peach-Koehler force term emerged in their model, a reliable solution of the stress-induced kink's configuration could not be obtained from their equation. David Rodney and Laurent Proville found a numerical solution for this problem by imitating the semi-discrete variational Peierls-Nabarro theory, they found the solution is metastable and the kink's height decreases along with the increasing applied stress (Proville et al., 2013; Rodney and Proville, 2009). However, in their method, the remote dislocation line was fixed on the Peierls valley under stress condition, which was not very natural in continuum physics. We will discuss this later. The FK model is a discrete form of line tension model bounded with the periodic conditions, and it seems to be realistic for producing a 2D phonon scatter on the compute cell naturally (Rodney and Proville, 2008). A discrete FKL model was proposed by T. D. Swinburne et al., which was able to reproduce the coarse-grained data of the diffusion of kinks with much less computation cost than MD work. They also proved that the long ranged kink interaction was a minor perturbation in the formation energy (Swinburne et al., 2013). In these models, the only remaining parameter to be found is the line tension which directly related to the dislocation line energy composing of the contribution from the elastic field and the dislocation core (Clouet et al., 2011). The orientation dependence of line tension is always omitted at a single slip system in these models, and the competitive relation among the line tension, the conservative force arising from the Peierls potential and the Peach-Koehler force arising from the applied stress field controls the equilibrium shape of the kink-pair.

The line tension theory is known to difficult to describe the Coulomb-type kink interaction from elasticity theory (Hirth et al., 1983). Though, some approximate methods are proposed to study the influence of the elastic interaction to the nucleation enthalpy of the kink-pair (Seeger, 1956; Seeger and Schiller, 1962), the full elastic field of the dislocation is not considered well. Thus, the elastic interaction models based on the dislocation-dislocation interaction theory are proposed to describe the kink mechanism (Eshelby, 1962; Hirth et al., 1983; Koizumi et al., 2006). In these models, at least two parameters need to be chosen appropriately for giving an accurate prediction of the activation energy of a well-separated kink-pair. One is the cut-off parameter of the dislocation core; the other is the stable kink's width. Both of them can be obtained from the atomic scale simulations (Koizumi et al., 2006). A. Kraych et al. investigated the kink mechanism in high pressure $MgSiO_3$ perovskite by using the elastic interaction model with the parameters adjusted to match the MD data (Kraych et al., 2016). The critical nucleation enthalpy was evaluated by the model successfully and their results seemed to support Hirokazu Koizumi et al.'s conclusion, that the nucleation enthalpy of the trapezoidal kink-pair obtained by using the elastic interaction model reproduced well the stress-dependent given by the line tension model, except at low stress.

We shall be interested here that the shape of Peierls potential to cause the dislocation to form a stable kink. A well-known kink solution obtained from the SG theory is the analytical base for describing the thermal activated kink configuration and can be used for judging the accuracy of MD works (Peyrard and Kruskal, 1984; Rodney and Proville, 2009). Focus on the $\langle 111\rangle\{110\}//2$ screw dislocation in BCC iron; the metastable core structure (the split core) indicates that there is a minimum Peierls barrier located between the two adjacent stable minima. For deriving a solution of the kink configuration on the camel-hump potential that a double SG equation, or a high order equation dependents on the local minimum's depth and location, is required to solve. Moreover, for deriving the stress-induced kink's configuration that a perturbed SG equation, which has no analytical solution yet, is required to solve (Hua and Liu, 2002). In order to avoid the complicated math work, a continuum model mimicking the dislocation phase field theory is presented and the order parameter is associated with the screw dislocation line's equilibrium location in a selected domain (Lee et al., 2011; Levitas and Javanbakht, 2015). The phase field model, to which the current work belongs, is based on the interface model from the three-dimensional Landau theory for stress-induced martensitic phase transformation (Levitas et al., 2003, 2010). DongWook Lee et al. developed this theory to