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ScienceDirect
International Journal of Plasticity 25 (2009) 361–377
INTERNATIONAL JOURNAL OF Plasticity
www.elsevier.com/locate/ijplas

Slip systems interactions in α-iron determined by dislocation dynamics simulations

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Received 3 September 2007; received in final revised form 22 December 2007
Available online 26 January 2008

Abstract

Dislocation–dislocation interactions are investigated in α-iron using dislocation dynamics (DD) simulations. Special attention is paid to the simulation conditions and parameters to reveal the domain of validity of the calculations. Interaction coefficients between the $\{1\bar{1}0\}\langle 111\rangle$ slip systems are computed and analyzed in connection with the dislocation microstructures developed during simulations. The so obtained crystalline law is used to predict the flow stress in a massive DD simulation of a tensile test in duplex slip condition.

Keywords: Plastic deformation; Strain hardening; Dislocation dynamics simulations; Dislocation interaction; Interaction coefficients

1. Introduction

The purpose of this paper is to determine, in a physically justified manner, constitutive parameters for a crystalline plasticity model dedicated to the low carbon steels used in reactor pressure vessels. These bainitic materials exhibit a specific morphology made of lathes of ferrite with second phase particles at the interfaces and in the lathes. This complex problem is in a first step simplified by considering single crystals of α-iron deformed in

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doi:10.1016/j.ijplas.2007.12.009

the reactor pressure vessel conditions ($T > 300$ K). The main physical features to be taken into account are (i) the presence in the initial state of a large density of dislocations (about 10^{14} m^{-2}) and, (ii) the existence of a high friction associated to solid solution elements.

In conformity with the forest model analysis in pure materials with low lattice friction (Saada, 1960; Kocks and Mecking, 2003), the flow stress τ and the dislocation density ρ are related by the Taylor relation, $\tau = \alpha\mu b\sqrt{\rho}$, where μ is the shear modulus and b the magnitude of the Burgers vector. In this formula, α is a well-known coefficient in the range 0.2–0.5, which defines the average strength of distribution of dislocations. The predictive ability of the Taylor relation is, however, limited since it lumps all densities into a single variable. Hence, this solution proscribes accounting for differences in the strength of dislocation microstructure that arise from differences in the slip system activities. For this reason, Franciosi et al. (1980) proposed a more sophisticated equation considering the contribution of individual slip system. The critical shear stress, τ_c^p, needed to activate a slip system p is then defined as

$$\tau_c^p = \mu b\sqrt{\sum_s a^{ps}\rho^s} \tag{1}$$

where the summation is carried out over all the existing slip systems 's' (including system 'p'). In Eq. (1), ρ^s is the dislocation density of individual slip systems and each coefficient of the interaction matrix a^{ps} define the average strength of the interactions between pairs of slip systems. The aim of the present work is the determination of such a^{ps} coefficients in the special case described above.

Eq. (1) is nowadays a standard ingredient for crystalline plasticity models. It was successfully used in finite-elements simulations for the plasticity of single crystals (Teodosiu et al., 1993; Tabourot et al., 1997; Hoc et al., 2004) or the description of grain deformation in polycrystals (Hoc et al., 2001; Evers et al., 2002). A precise evaluation of the a^{ps} matrix is a key parameter of such modeling. For instance, it was found that in the case of f.c.c. single crystals, the orientation dependence of the 'stage I' observed on the stress–strain curves of single crystals is strongly dependent on the amplitude of the a^{ps} coefficients (Hoc et al., 2004). Moreover, the exceptional value of one coefficient attached to the interactions between slip systems sharing the same Burgers vector (the collinear reaction), has provided an explanation to the long standing question of slip systems selection or exclusion in multi-slip conditions (Madec et al., 2003a,b; Devincre et al., 2005).

Attempts have been made to directly correlate individual dislocation–dislocation reactions to the interaction strength between slip systems at a larger scale. Following the seminal work of Saada (1960), Schoeck and Frydman (1972) calculated the stability of several elementary configurations based on line tension approximation. From this work, conclusion is made that the macroscopic response of a large density of dislocations cannot be precisely integrated starting from the analysis of individual forest reaction. Latter, such a conclusion was even consolidated by the work of Wickham et al. (1999) who reported the existence of a new forest reaction: the crossed-state. In recent years, the domain of occurrence of crossed-states as well as all the other elementary forest reactions in f.c.c. and. b.c.c. crystals has been systematically studied with dislocation dynamics (DD) simulations (Wickham et al., 1999; Kubin et al., 2003; Madec and Kubin, 2004; Shenoy et al., 2000). These simulations and analytical calculations based on line tension approximation (Dupuy and Fivel, 2002) have evidenced one additional problem. The length and the strength of forest junctions are strongly stress dependent. This is why, one can conclude