ELASTIC INTERACTION BETWEEN A DILATATION CENTRE AND SPLIT DISLOCATIONS IN B.C.C. METALS

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The elastic interaction energy between a dilatation centre and ½[111] dislocation split on {110} planes in b.c.c. metals is calculated for sessile and planar splittings of screw dislocation and for planar splitting of edge dislocation; the splitting is considered as a model of the dislocation core. It is concluded that the interstitial impurity atom has three or four possible minimum energy positions in the dislocation core. A hypothesis on the impurity jumps in the dislocation core is proposed.

1. INTRODUCTION

Some aspects of interaction between the point defects and dislocations can be described within the continuum model (for a review, see e.g. [1, 2]). Recently, the elastic interaction between the point defects and split dislocations has been treated for f.c.c. metals [3, 4, 5].

In this paper, a simplified special case of the short-range interaction between the point defects and dislocations in b.c.c. metals will be discussed. In general, the structure of both the interacting defects should be taken into account.

The structure of the dislocation core can be described, in the first approximation, by the dislocation splitting. However, the stacking fault energies in the b.c.c. metals seem to be very high and the dislocations cannot be considered as distinctly split as e.g. in f.c.c. metals. Nevertheless, different splittings of dislocations in b.c.c. metals on {110} and {112} planes have been proposed and to some extent justified by recent computations of the atomic core structure (for a review, see e.g. [6]). However, the effective width of splitting is very small, of the order of a few interatomic distances, and the splitting should only be considered as a continuum model of the dislocation core which describes well the core symmetry.

The structure of point defects can be roughly described, within the continuum approach, as a region which has different elastic constants from the matrix (“modulus effect”) or/and which undergoes dilatation or tetragonal distortion (“size effects”) [1, 2]. For interstitial impurity atoms of carbon or nitrogen in alpha-iron, the previous studies have considered as dominating the dilatation effect for interaction with non-split edge dislocations [7] and the tetragonal distortion effect for interaction with non-split screw dislocations [8]. Recently, the interaction of tetragonal distortion centres with screw dislocations split on {112} planes has also been studied [9, 10].

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In this study, the point defect will be described simply as a dilatation centre. The linear isotropic theory of elasticity will be used and, therefore, the dilatation centre will interact with the edge components of the individual partials only. The elastic interaction energy $E$ between the dilatation centre and the split dislocation can then be written as a sum

$$E = A \sum_{i=1}^{n} \alpha_i f_i,$$

where $A = \frac{1}{3} \frac{(1 + \nu)}{(1 - \nu)} Gb R^3 \delta$, $G$ is the shear modulus and $\nu$ the Poisson ratio, $b$ the value of the Burgers vector of the complete dislocation, $\delta$ the unrelaxed dilatation, $\delta = (R - R')/R$, $R$ is the radius of the spherical hole into which a sphere of radius $R'$ and of the same material is inserted; $\alpha_i = b_i^0/b$, $b_i^0$ is the value of the edge component of the $i$-th partial in units $b$ and $f_i = \sin \theta_i/r_i = y_i/(x_i^2 + y_i^2)$ where $r_i, \varphi_i$ and $x_i, y_i$ are the polar and cartesian coordinates, respectively, of the dilatation centre connected with the $i$-th partial (parallel to the $z$-axis) with $x_i$ chosen in the $b_i$ direction. The interaction of the dilatation centre with the stacking fault ribbons is neglected.

For b.c.c. metals, $b = a/2 [111], b = a \cdot \sqrt{3}/2$ where $a$ is the lattice parameter. Only the splittings on the $\{110\}$ planes corresponding to the stacking faults of the $a/8 \langle 110 \rangle$ type will be assumed so that the number of partials will be $n = 3$ for planar splittings $[11]$ and $n = 4$ for a sessile splitting of a screw dislocation $[12]$.

2. INTERACTION ENERGY

2.1. Screw dislocation split on three $\{110\}$ planes

A screw dislocation in the low energy sessile configuration can be split on three planes of $\{110\}$ type of the $[111]$ zone into four partials according to the reaction $[12] b = b_1 + b_2 + b_3 + b_4$ where $b_1 = a/8 [110], b_2 = a/8 [101], b_3 = a/8 [011], b_4 = a/4 [111]$ (see Fig. 1). Their edge components are $b_1^* = a/24 [112], b_2^* = a/24 [121], b_3^* = a/24 [211], b_4^* = 0$ so that $\alpha_1 = \alpha_2 = \alpha_3 = \sqrt{2}/12 = 0.118 = \alpha, \alpha_4 = 0$: the central dislocation is pure screw and does not interact with the dilatation centre. In equilibrium, the three side partials are at distance $c$ from the central partial, $c = Gb^2/2\pi \cdot (15 - 16\nu)/144(1 - \nu) \cdot 1/\gamma$, where $\gamma$ is the stacking fault energy $[12]$.

The interaction energy $E$ can be written in the polar coordinates $r, \varphi$ connected with the central partial (Fig. 1) as

$$E = \frac{\alpha A}{c} \frac{3\varphi^3 \sin 3\varphi}{q^6 - 2q^2 \cos 3\varphi + 1},$$