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THE INFLUENCE OF THE TEMPERATURE ON THE PEIERLS ENERGY OF A $\frac{1}{2}<111>\{110\}$ EDGE DISLOCATION IN B.C.C. IRON CONTAINING IMPURITY ATOMS

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In the past, scant attention was paid to the interaction between dislocations and impurity atoms in computer simulations, in spite of the obvious importance of such interactions for the mechanism of plastic deformation. Moreover, comparatively little attention has been paid to dislocations of non-screw orientation. There is good evidence from electron microscopy and slip lines that edge dislocations are much freer to move than screw dislocations (1) (2) (3). Micro-strain measurements (4) indicate that there may be a threshold stress required to move edge dislocations (5) : if so, edge dislocations are not completely free to move.

Investigations (6) of the temperature and strain rate dependences of the yield stress and flow stress in iron have indicated that its plastic deformation occurs by thermally activated mechanism.

Sleeswyk (7) suggested a transition in the activation energy for dislocation glide on the $\{110\}$ plane analyzing the experimental observations on dislocation mobility at various temperatures obtained by Turner and Vreeland (6). The method of analysis is based on the following equation:

$$H(\sigma) = k T \ln \frac{v_c}{v}$$  

where the stress ($\sigma$) dependent activation enthalpy $H(\sigma)$ is related to the Boltzmann constant $k$, the absolute temperature $T$, the shear wave velocity $v_c$ and the dislocation velocity $v$. The experimental data points obtained at various velocities and temperatures are plotted in a $v$ vs. $kT \ln(v_c/v)$ diagram. The analysis pointed out that the activation enthalpy for the glide process on the $\{110\}$ plane in b.c.c. Fe at $77^\circ K$ is half of that of glide at and above $200^\circ K$. A computer simulation study is set up to explain this phenomenon by calculating the influence of the temperature on the Peierls energy of a $\frac{1}{2}<111>\{110\}$ edge dislocation in $\alpha$-Fe.

The first step in defect simulation is the construction of a large computational block by submitting each atom in it to the displacements predicted by anisotropic elasticity theory (8) (9). The crystallite is composed of fourteen $\{112\}$ planes in order to be able to embed a multiple of six planes in the elastic continuum. Additionally, these initial positions have been determined and the resolution of the simulation is assumed to be that the atoms will relax to final positions under the influence of a pair-wise interatomic interaction function as developed by Johnson (10). The displacements during the relaxation process have been calculated using Gibson’s integration procedure (11). The configuration is periodically “quenched” when the kinetic energy attains a maximum according to the method of Bullough and Perrin (12).

After the lattice had been relaxed the potential energy of a carbon atom was calculated for a grid of positions separated by 0.3 $\AA$ within a block around the dislocation core which extended over six planes in the $<112>$ direction. In this way the carbon atom at the place

The atomic configuration of one (112) plane in α-Fe of the relaxed crystallite containing an edge dislocation with Burgers vector $\frac{1}{2}[1\overline{1}1]$.

The potential energy (13) (14) is a minimum was found at the position of the distorted octahedral site between two consecutive (112) planes. The position of the carbon atom $C_1$ in the minimum is indicated in Fig. 1 as projected on a (112) plane.

Although calculations of the Peierls energy for dislocations have been carried out frequently in none of these the influence of impurities on the Peierls stress has been considered. The Peierls stress and Peierls energy have been calculated in this work for the dislocated lattice containing a carbon atom at site $C_1$ as illustrated in Fig. 1. The origin of the dislocation was displaced over a distance $\frac{1}{2}b$ in the $[1\overline{1}1]$ direction (9). The crystallite was relaxed for all intermediate steps along this direction.

It may be noted that so far the temperature of the lattice has not been involved in the model used. A molecular dynamical type of calculation (15) was applied to study the influence of the temperature on the Peierls energy and the Peierls stress as well. The method is based on the condition, valid for thermal equilibrium in a classical system of coupled oscillators that the mean kinetic energy of the system is equipartitioned among three degrees of freedom and that the velocity distribution is a Maxwell distribution. The lattice was first relaxed statically to a configuration of minimum energy, corresponding to the condition $T=0$ K. The temperature was given to the lattice by assigning a Maxwell distribution to the velocity components of the atoms in a random order. The lattice points were allowed to move. The total energy $3kT$ became quickly distributed between the kinetic and potential energies of the lattice. The time needed for the distribution was equal to 10 time steps $\Delta t$ during the relaxation process ($10\Delta t = 10^{-13}$ s), or approximately one period of atomic oscillation at the Debye frequency. The lattice temperature can then be defined by the mean kinetic energy of the lattice ($= 3kT/2$).

Fig. 2 shows the Peierls barriers for the motion of the $\frac{1}{2}[1\overline{1}1](110)$ edge dislocation containing a carbon atom at 70°K as well as 200°K. The energy difference is given per unit periodicity length ($2\sqrt{2}$) along the dislocation line in the $<112>$ direction. The Peierls stresses which correspond to the Peierls barriers are in both cases lying between $0.008\mu$ and $0.009\mu$, where $\mu$ represents the shear modulus for the shear on a $[110]$ plane in the $<111>$ direction.
Potential barrier encountered by a $\frac{1}{2}[111] \{110\}$ edge dislocation in $\alpha$-Fe containing a carbon atom and moving in the $<111>$ direction over a fraction of the Burgers vector, corresponding to $T=70^\circ K$ (•) and to $T=200^\circ K$ (○).

It may be noted that the diagram of the Peierls energy calculated at $70^\circ K$ is similar to the curve in the case of $0^\circ K$, published elsewhere (16). Further, in Fig. 2 an intermediate state at 0.2b is depicted in the case of $70^\circ K$. The increase of energy is then equal to 0.028eV per unit periodicity along the dislocation line. The intermediate maximum is equal to 0.032eV and the absolute maximum is equal to 0.053eV. The secondary maximum in the Peierls energy does not appear at $200^\circ K$. The transition in the activation energy for dislocation glide on a $\{110\}$ plane can be explained by this secondary maximum in the Peierls energy curve which is present at $70^\circ K$ and which does not exist at $200^\circ K$. The calculations carried out for a dislocated lattice without any carbon atom, did not produce any secondary maximum in the Peierls energy (16).

Under the condition of constant volume produced by fixed boundaries during the relaxation process, the pressure in the lattice may be expected to increase with increasing temperature. We assume that the effect of pressure on the motion of line defects would be small. Moreover, the use of anharmonic interaction potentials entails a perturbation in the equipartition of the kinetic and potential energies. The influence of the pressure means only a small effect on the results compared with the more serious approximation made by using pair-wise interaction functions.

Recently, Kuo and Arsenault (17) determined the interaction force between a straight edge dislocation moving through a three dimensional block containing solute atoms. It was assumed that the solute atoms are located randomly in the lattice. Therefore, any strengthening due to short-range order is not accounted for. Moreover, the influence of the temperature on the Peierls energy was not taken into account.

Another method to calculate the Peierls energy has been introduced by Basinski (18) by applying an external stress on a crystallite containing a screw dislocation. Larger stresses were built up by application of small increments until a critical stress was reached. Alternatively, Sinclair (19), Gehlen et al. (20) have each presented a flexible boundary scheme. In these methods the coordinates of the atoms at the boundary are periodically repositioned as the inside of the block, containing the 'free atoms', is relaxed. The atomistic calculation of the Peierls energy of a $\frac{1}{2}[110]$ edge dislocation in MgO by Puls et al. (21) shows the likely constrains on the core structure calculation associated with the use of rigid boundary conditions. Despite its limitations, we have chosen to calculate the Peierls energy.
using rigid boundary conditions. The considerably greater complexity of the method of Sinclair makes it less suitable in a first attempt to investigate the influence of the temperature on the Peierls energy.

We may conclude that the results presented here appear to be in reasonable agreement with the experimental data. The explanation of the experiments is not based on a dissociation into $\frac{1}{4}[111]$ partial dislocations as has been suggested by Sleeswyk (7). Another plausible explanation could be the effect of impurity atoms on the Peierls energy at various temperatures. The present computer simulation study is a beginning; the next step is to consider the influence of the fixed boundaries on the results.

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