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COMPUTER ANALYSIS OF A SLIP MOTION OF A SCREW DISLOCATION IN A BCC LATTICE

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Slip motion of a screw dislocation in a bcc lattice under shear stress was simulated and analyzed using an atomicrow potential (two dimensional calculation) and Johnson potential (three dimensional calculation) for three typical direction of shearing, i. e., $\chi=-30°$ (twinning direction), $\chi=0°$ and $\chi=30°$ (anti-twinning direction). In the case of an inter-atomicrow potential yield stresses were obtained as 3×10^{-3}, 4×10^{-3} and $28\times10^{-3}\mu$ for the above three directions, respectively ($\alpha=0$) and 23×10^{-3}, 21×10^{-3} and $26\times10^{-3}\mu$ for $\alpha=0.1$. Slip planes obtained in these calculations were twinning (112) plane, except the antitwinning stressing in $\alpha=0.1$, where (101) slip was activated. For these two types of potentials metastable configurations at half an atomic distance were not obtained and the stable core structure was a polarized type (degenerate type).

In the case of Johnson potential for iron the stable core structure was an unpolarized type (non-degenerate type) and a metastable configuration at half an atomic distance was obtained. The calculated yield stress was very high in this case, $88\times10^{-3}\mu$ for the twinning direction.

Key words: Computer simulation, Screw dislocation, Core structure, Slip motion, BCC metal

1. Introduction

To investigate the intrinsic plastic behaviours of bcc metals, a number of computer works have been performed on the atomic configuration of the screw dislocation core in a bcc lattice and its motion under

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applied stress using the assumed interatomic or interatomic-row potentials (1–12). Suzuki calculated the two-dimensional Peierls potential map for a screw dislocation using a simple interatomic-row potential, obtaining a Peierls stress which is about one order of magnitude higher than that of experimental results (1). After this work, the direct application of shear stress to a model bcc lattice which contains a screw dislocation was performed to obtain the Peierls stress and the core structure under stress by many investigators, e. g., Vitek (2,3), Yamaguchi (4), Basinski (11), Minami, Kuramoto and Takeuchi (5, 6, 7, 8), Takeuchi (9, 10) and Masuda and Sato (12). Values of Peierls stress obtained are scattered in the range of (1∼5) τ_p^e, where τ_p^e is the Peierls stress obtained in the experiments. The absolute value of the Peierls stress is not so important because of the uncertainty of the interatomic potential used, but the slip plane obtained in the simulation is more important when compared with the experimental results. Most of the calculations showed the twinning $(\bar{1}\bar{1}2)$ slip plane for a motion of a screw dislocation under shear stress and the type of core structure was a polarized one. This result explained the experimental results for less pure tantalum (13), less pure molybdenum (14). The orientation dependence of the yield stress at low temperatures is another important factor which must be explained by calculation. The experiments showed the monotonously increasing relation between the yield stress τ_y and χ while the calculation also gave same tendency. Then until the date of around 1976 it was roughly regarded that the computer simulation accomplished the initial purpose. However, in the last five years the situation has been changed again to a final goal of plastic behaviours of bcc metals at low temperatures.

The most striking change has been given from the experimental results for high-purity single crystals of iron and molybdenum (15, 16, 17) at very low temperatures, especially at 4.2 k, namely, a concave type $\tau_y-\chi$ curve and $(\bar{1}01)$ slip plane were given from these experiments in stead of a monotonously increasing type $\tau_y-\chi$ curve and $(\bar{1}\bar{1}2)$ slip plane in the previous results, respectively. Moreover, a hump on τ_y-T curve was recognized clearly for iron and molybdenum. These drastic developments stimulated the computer simulation again and the new features appeared in some points, namely, i) an unpolarized type core structure which has a metastable configuration at half an atomic distance was reconsidered to be important to explain the actual situation (15, 16, 17, 9, 10). ii) The $(\bar{1}01)$ slip appeared clearly in the computer simulation for some interatomic potentials used. Especially the recent calculation which takes into account the contribution from d-electrons (Masuda and Sato (12)) also showed these new features.

In this report the possibility of $(\bar{1}01)$ slip and a metastable configuration were studied in two dimentional calcuation using a sinusoidal type

potential and in three dimensional calculation using Johnson potential.

2. Computation Procedures

The model bcc lattice used was the same as that in the previous calculation (5) shown in Fig. 1, where the view of bcc lattice from [111] direction is drawn. The lattice is almost square of $34\,b \times 34\,b$ and the number of an atomic row is 1570. In this rectangular block a screw dislocation is put in based on a linear elasticity, and the whole crystal was relaxed with a fixed boundary condition. and then the whole crystal was sheared to a certain strain and again relaxed fully. Thus the response of a screw dislocation for an applied stress was obtained. In these calculations, the convergence condition was adopted such that the displacements of any atomic rows were less than $5 \times 10^{-5} b$ in successive iterrations. Shear stress was applied in the [111] direction in $(\bar{1}01)$ plane, and in the twinning and anti-twinning directions in the $(\bar{1}\bar{1}2)$ plane. The core structure is shown by the differential displacement representation employed by Vitek (2), where the relative displacements along z-

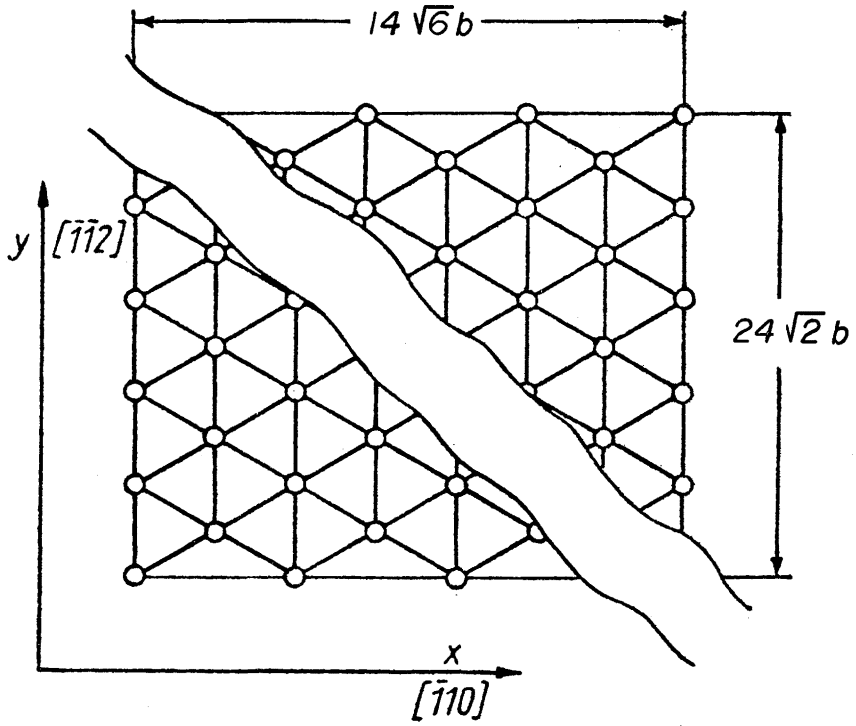

Fig. 1. The crystal block used in the present calculation viewed along the Burgers vector. Circles indicated atomic rows.

axis between the nearest atomic rows with respect to the status of the perfect crystal are indicated by arrows.

3. Results

In Figs. 2, 3, 4, 5 results of two dimensional calculation using an interatomic-row potential denoted in Fig. 2 are shown. Figs. 2 and 4 give $\phi-\chi$ and $\tau_p-\chi$ curves for $\alpha=0$ and 0.1, respectively, where ϕ is the angle between the actual slip plane and $(\bar{1}01)$ and χ is the angle between the maximum shear stress plane and $(\bar{1}01)$, and α is the parameter in the potential. In Fig. 2 the dotted line shows the result of free boundary condition, which is slightly different from that obtained from the fixed boundary condition. So all the calculations hereafter were performed with the fixed boundary condition. The Peierls stress is, roughly speaking, an increasing function of χ, except the second yield stress τ_2 in Fig. 4, where τ_1 and τ_2 are the stresses for the preyielding and the actual yielding. The pre-yielding means the change from the initial configuration to the split configuration. The detailed core structure changes under increasing applied shear stress are shown in Figs. 3 and 5 for $\alpha=0$ and 0.1, respectively. Each figure shows three sequences from up to down for three directions of applied shear stress. The actual slip plane is twinning $(\bar{1}\bar{1}2)$ plane as shown in these figures except $\chi=30°$, antitwinning shearing. The twinning $(\bar{1}\bar{1}2)$ slip is very easy to understand because a screw dislocation core has a polarized type structure as shown at the top of these figures, zero applied stress. The polarized core should have a zigzag path connecting two $(\bar{1}10)$ planes making 60° under the shear stress, e. g., $\chi=-30°$ in Fig. 3, and the resulting path is $(\bar{1}\bar{1}2)$ slip plane. This is a well-known pattern of a motion of a polarized core, namely, changing the sense of polarization alternatively. But for $\chi=30°$ the antitwinning $(\bar{2}11)$ slip and $(\bar{1}01)$ slip occurred for $\alpha=0$ and 0.1, respectively. The former is a zigzag path but not so simple as that in $\chi=-30°$, and the latter is a rare case for this type of potential. As shown in Fig. 5 $(\bar{1}01)$ slip shows a somewhat complicated core structure change during motion, namely, motion with a deformed area ahead, which seems just like a microtwin. For both potentials $\alpha=0$ and 0.1 no metastable configuration at half an atomic distance was observed.

In Figs. 6, 7 and 8 the results of three dimensional calculation using the so-called Johnson potential for iron (18) are shown. As shown in Fig. 6 and 7 a screw dislocation has an unpolarized (isotropic) core structure in this case and a metastable configuration at half an atomic distance is observed as shown in Fig.8. But Peierls stress is very high, and unfortunately they have not been determined yet as shown in Figs.

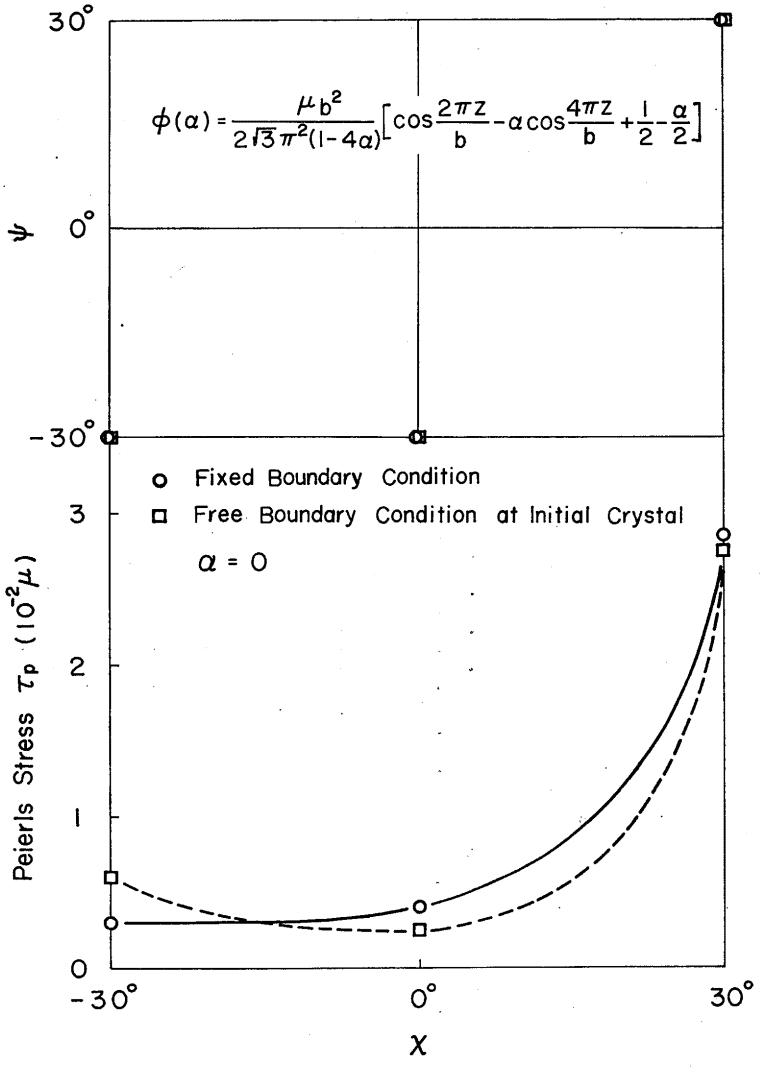

Fig. 2. Calculated τ_y—χ and ψ—χ relations for the interatomic-row potential with α=0.

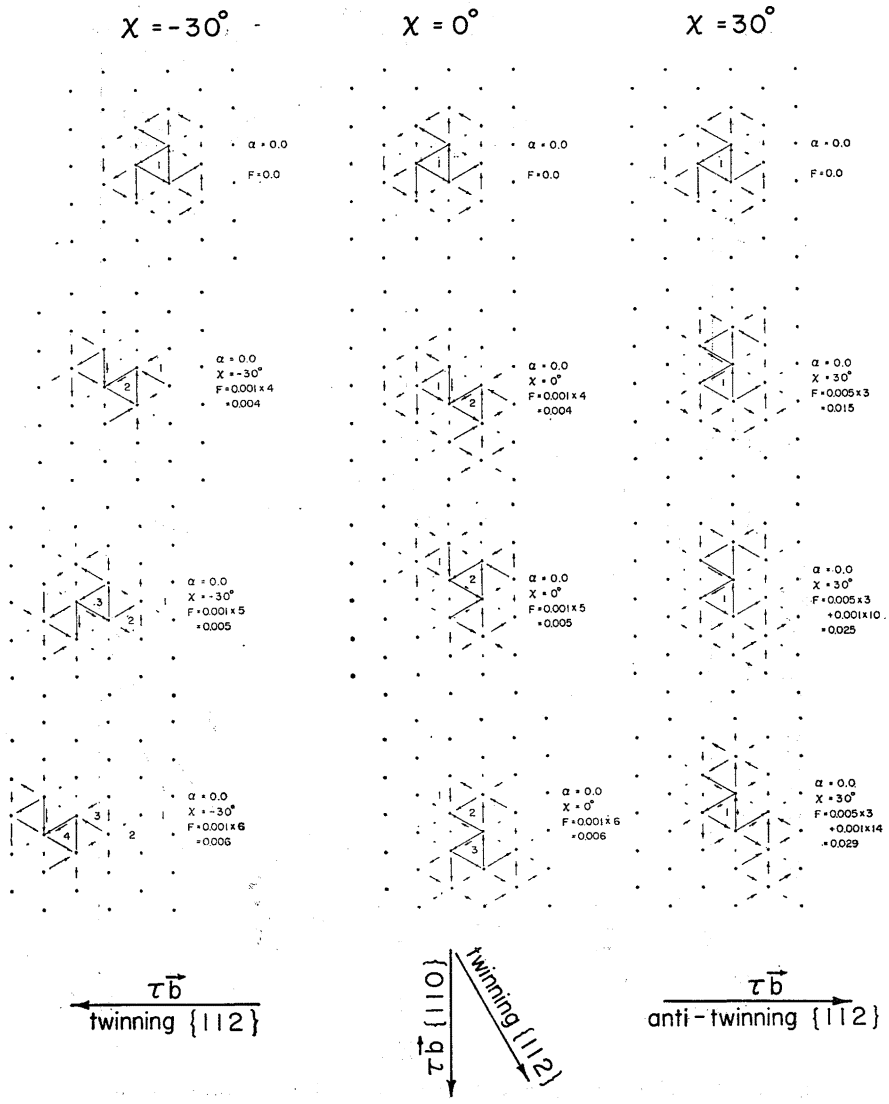

Fig. 3. Successive translations of the dislocation under the applied shear stress (stress increasing from top to bottom) for three different directions. (α=0 potential).

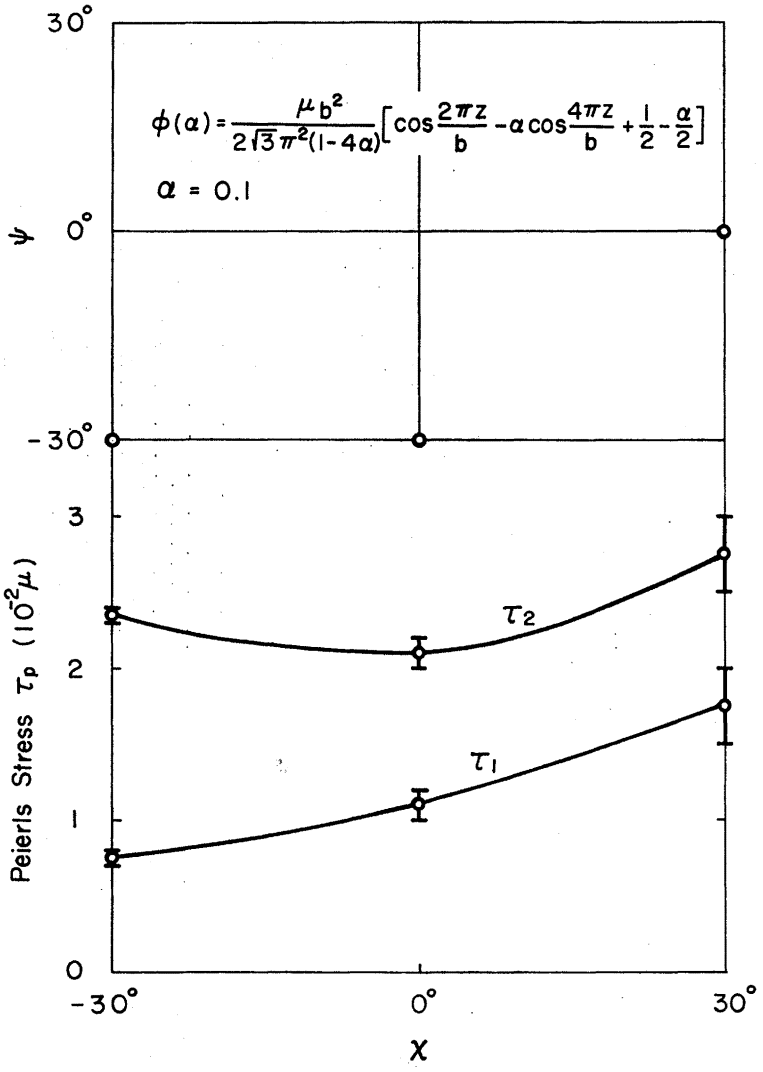

Fig. 4. Calculated τ_p—χ and ψ—χ relations for the interatomicrow potential with α=0.1.

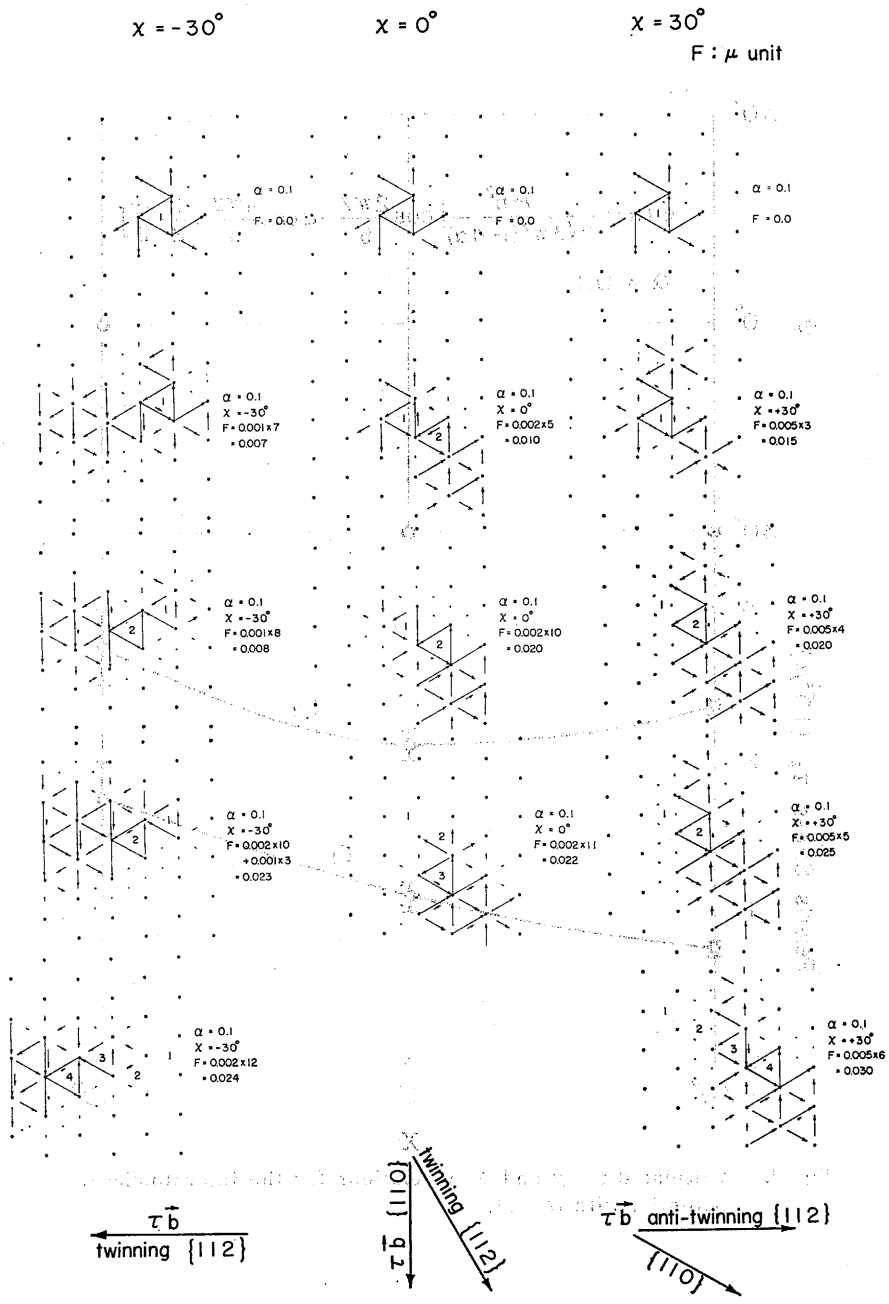

Fig. 5. Successive translations of the dislocation under the applied shear stress (stress increasing from top to bottom) for three differerent directions. (α=0.1 potential).

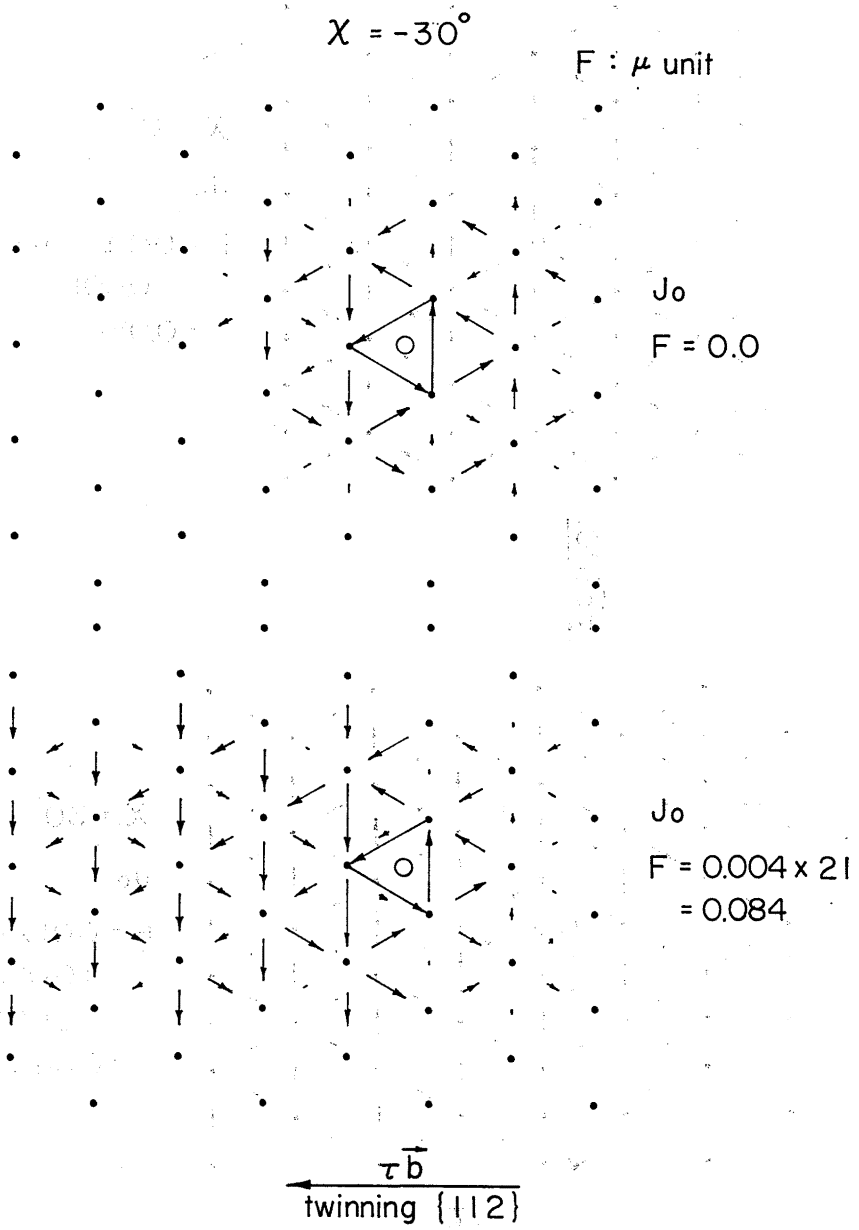

Fig. 6. Calculated core struture under various stress applied for three different directions using Johnson potential.

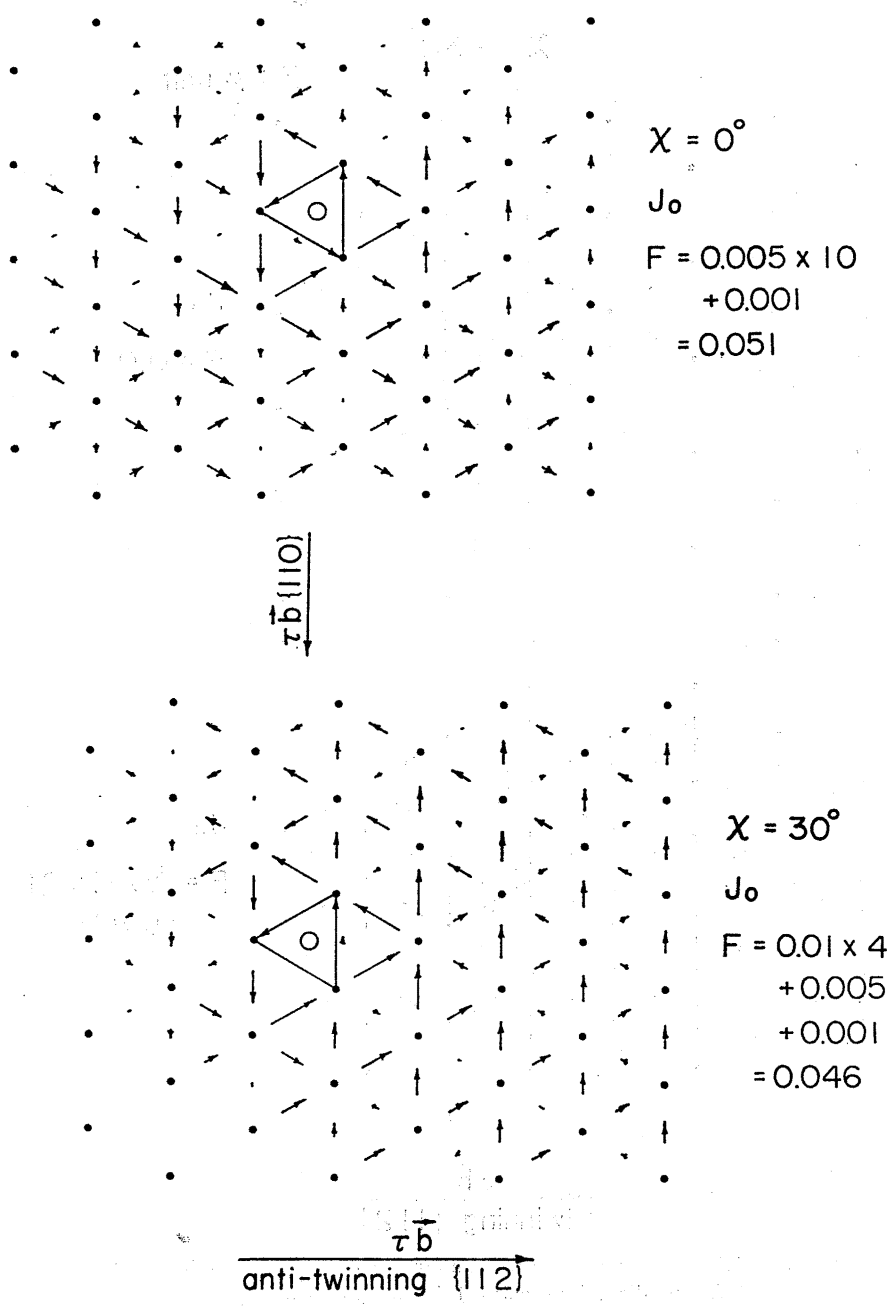

Fig. 7. continued from Fig. 6.

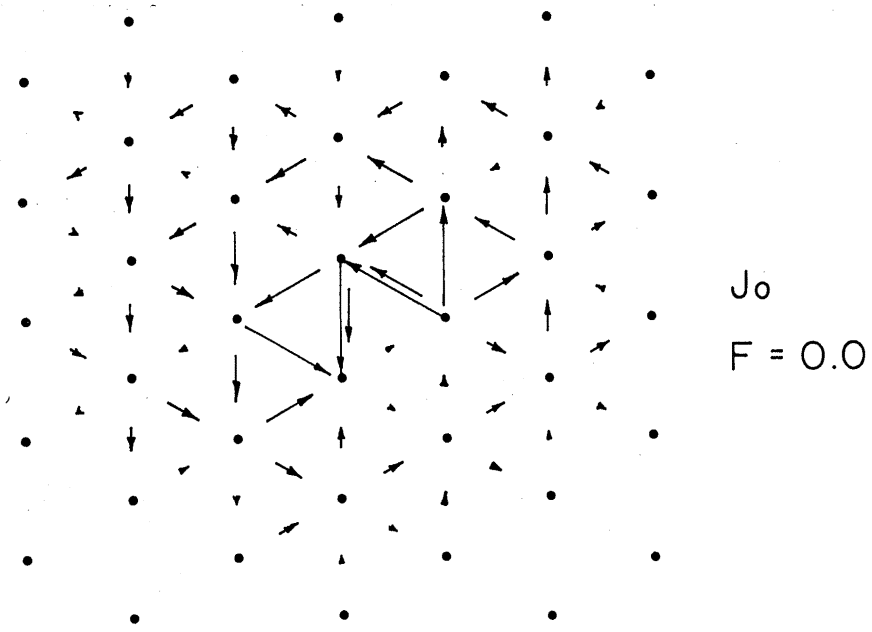

Fig. 8. A metastable configuration of a screw dislocation core obtained by Johnson potential.

6 and 7 for all the directions.

4. Discussion

As mentioned in section 1 recent experimental results using high-purity bcc metals show ($\bar{1}01$) slip, a hump on $\tau_y - T$ curve and a concave type $\tau_y - \chi$ curve (15, 16, 17) at low temperatures. A hump can be explained by the existence of a metastable configuration of a screw dislocation core at half an atomic distance (16, 18). From these standpoints it is concluded that the calculated results using an interatomic-row potential ($\alpha = 0$ and 0.1) cannot explain the expermiental results because they do not show the metastable configuration, though sometimes ($\bar{1}01$) slip can be predicted. On the other hand, three dimensional calculation using Johnson potential shows the metastable configuration, so it has a possibility to correspond to the actual experimental results, though ($\bar{1}01$) slip has not been obtained yet. Johnson and Wilson (18) calculated the migration energy of a vacancy in iron using this potential and obtained a small value 0.71 eV, which was considered to be too small when presented. But very recently several experimental results which support this small migration energy appeared, e. g., positron annihilation lifetime

measurements in high-purity iron (19, 20) and irradiation experiments in a high voltage electron microscope using high-purity iron (21). These suggest that Johnson potential gives a fairly good result in the migration of a vacancy in iron. It is then expected that Johnson potential can give a good result in a calculation of a core structure of a screw dislocation in iron and its motion under stress. In the early date, Vitek (3) did not use an original Johnson potential because it gives a very high Peierls stress. But the absolute value of the Peierls stress is not a most important factor, but a type of core structure and its behaviour under stress, stability of a split configuration (metastable configuration) are

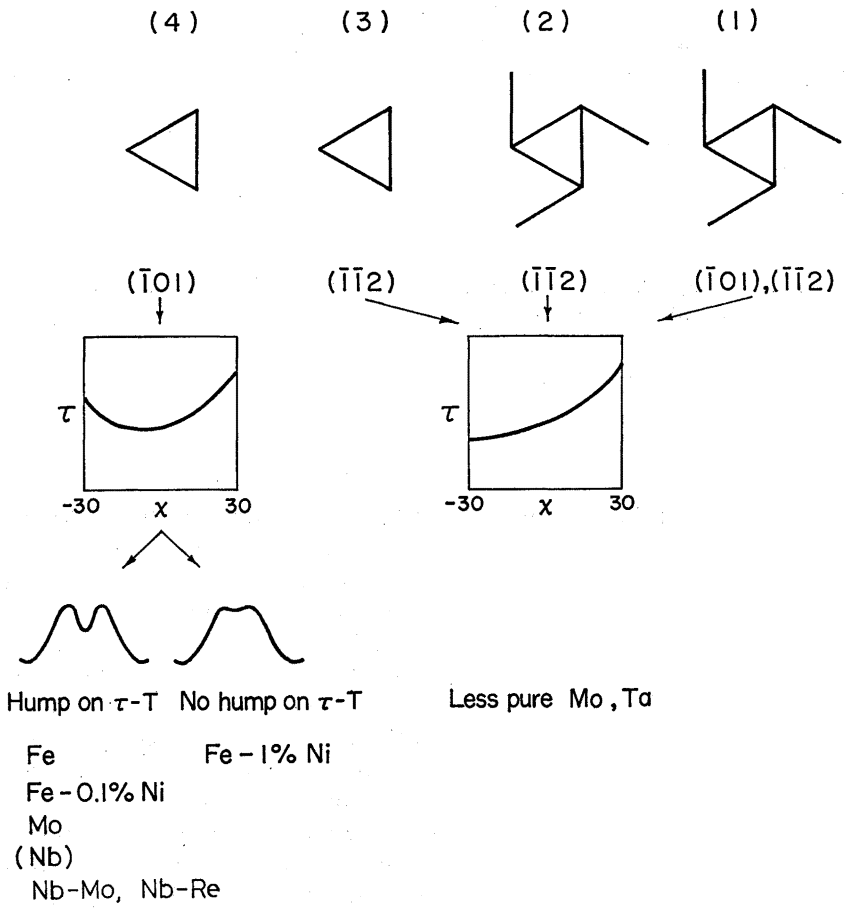

Fig. 9. Four types of combination of screw dislocation core and slip plane proposed by Takeuchi, (4) is considered to correspond to actual bcc metals shown in figure.

more important factors. From these viewpoints it should be stressed that Johnson potential has a possibility to explain the low temperature plastic behaviours in iron and so more detalied analysis will be required to reach the good accordance between the experiments and calculations.

The recent Takeuchi's calculation (10) shows roughly four types of combinations of core structure and slip plane as shown in Fig. 9, although this calculation uses very empirical interatiomic-row potentials. The important point is that the type (4) is the most favorable type to explain the actual experimental results, because (4) gives an unpolarized core which has a metastable configuration and shows $\bar{s}$ (101) slip.

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