ON THE MOTION OF DISLOCATION BENDS IN TERMS OF THE KINK MODEL

H. Gottschalk

To cite this version:


HAL Id: jpa-00223077
https://hal.archives-ouvertes.fr/jpa-00223077
Submitted on 1 Jan 1983

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L’archive ouverte pluridisciplinaire HAL, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d’enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.
ON THE MOTION OF DISLOCATION BENDS IN TERMS OF THE KINK MODEL

H. Gottschalk
Abt. f. Metalphysik, II. Physikalisches Institut, Universität Köln, Ulmicher Str. 77, D-5000 Köln 41, F.R.G.

Résumé - Le régime permanent de déplacement des parties courbées des dislocations dans un cristal de silicium en cours de déformation est expliqué par un modèle de décrochements dans lequel les décrochements s'annihilent au voisinage de l'apex de la courbure. On discute le paradoxe apparent d'une déformation sous faible contrainte conduisant à des dislocations courbées malgré un potentiel de Peierls élevé.

Abstract - The steady state motion of dislocation bends in silicon taking place when the crystal is being deformed is explained in terms of the kink model assuming a kink annihilation mechanism in the apex region of the bend. The apparently paradoxical behaviour that a deformation at low stress produces curved dislocations though the Peierls energy is high is discussed.

After the deformation of silicon crystals under high stress at low temperature one typically finds straight dislocation segments lying in the $<110>$-Peierls troughs. The dislocations contain bent segments when turning from one $<110>$-direction to another one. The observations are still the same changing to lower stress and higher deformation temperature, provided the local dislocation density is not too high (see Fig.1 and Fig.3 in /1/).

It is remarkable that it is possible to calculate the applied stress from the measured radii of curvature of the bends in specimens cooled to room temperature with applied load. In these specimens the dislocations are therefore imaged in the state of moving. The assumption that the resolved shear stress and the backstress exerted by the line tension in the bend are equal therefore seems to be justified /1/.

An easily seen consequence of a steady state motion of a dislocation bend is that the dislocation velocity of each segment of the bend is only dependent on the velocities of the two adjacent straight segments and a geometrical relation but independent on the actual stress in the bend and the character of the segment in question.

Considering the dislocation motion in a diamond-like semiconductor as performed by the nucleation and the sideways motion of kinks there arise some questions concerning the behaviour of kinks in the bent dislocation segments.

In the concept presented here the dissociation of dislocations is not considered in particular. For low stress and small dislocation splitting the motion of kinks on both partials is correlated, then the dislocation can be treated like a perfect one. For high stress and wide splitting when the kink motion is uncorrelated, the concept may be applied to each partial separately.

First, suppose a static dislocation bend with radius of curvature $R$ (Fig. 1). To establish a 60°-dislocation bend a certain number and a certain distribution of kinks on the dislocation is necessary. Assuming that the bent segment $A_1A$ is formed of kinks belonging to segment 1 and $A_2A'$ of kinks belonging to segment 2, a simple geometrical consideration yields the total number $Z$ of kinks contained in the bend $A_1A'$.
\[ Z = 2 \left(1 - \cos 30^\circ\right) \frac{R}{a} = 0.27 \frac{R}{a} \]

(a is the distance of neighbouring Peierls troughs. \(a(Si) = 0.33\text{nm}, R = 100\text{nm}\) yields \(Z = 82\)).

The local distance \(y\) of kinks depends only on the angle between the average dislocation line and the \(\langle 110\rangle\)-direction:

\[ y = \frac{a}{\sin \beta_i}, \quad i = 1, 2 \quad \text{(see Fig.1)} \]

and the local kink density:

\[ z = \frac{1}{y} = \frac{\sin \beta_i}{a} \]

these values both being independent of \(R\). As \(\beta_1^\text{max} = 30^\circ\),

\[ y_\text{min} = 2a, \quad z_\text{max} = 1/2a. \]

The kinks present in the segment \(A_1A\) are all kinks with the same sign. Hirth and Lothe /2/ have shown that there exists a mutual repulsive force of kinks of the same sign and that the force exerted by the line tension of a bent dislocation segment can be derived from this kink-kink interaction.

Considering the apex of a bend one notices (Fig. 2) that it is by no means possible to reduce the distance of neighbouring kinks below the minimal length \(2a\) because of crystallographic reasons. It can be seen, too, that the two sorts of kinks, e.g. BC (or ABCD) on segment 1 and CD (or BCDE) on dislocation 2 cannot be distinguished.

The consequence of the dynamic equilibrium state of a moving bend arrangement is that the total number of kinks lying in the bend and the local kink density must be constant by time. When kinks driven by the applied stress are approaching the bend they must slow down by the effect of the repulsive forces of the kinks still present in the bend. Simultaneously they exert forces on all kinks of the bend, which will move a small distance towards the apex. A differential change of the kink distance in the apex region, however, is no longer possible. The force on the apex kinks is increasing by new kinks joining the bend until a kink of double height (Fig.2, \(C \rightarrow C', \text{new line} AC'E\)) may be generated and the whole configuration is rearranged. This process is equivalent with the annihilation of a kink.

This concept is in good agreement with experimental results obtained for dislocations moving under low stress and for the leading partials in high stress deformed crystals /1/. Interesting, however, is that the radii of curvature for the trailing partials in the high stress deformed crystals in general are found too large, so that the force exerted by the line tension is less than the applied driving force. Perhaps particularly the trailing partial has strong interaction with point defects which make the annihilation of kinks in the apex region more difficult. To overcome these obstacles an increasing number of kinks is piled up in the bend, the force exerted by the line tension decreases, and part of the driving force is now present to stimulate the kink annihilation process.

The relaxation of a frozen in dislocation formation may be considered within the same framework. From experiments it is known that in general the radii of curvature are increasing when the system is relaxing /3/. Here two limiting cases must be distinguished: the split dislocation with small separation and the isolated partial.

In the first case the stress acting on the straight segments nearly vanishes and only the force exerted by the line tension is acting on the apex of the bend. In the
latter case the force acting on the straight segments is the stacking fault energy while in the bend the line tension is additionally effective. In both cases first a sideways motion of kinks from the apex may take place (Fig.3, full line changing to pointed line) and then a new kink may be created by reversing the annihilation process described before \((A\rightarrow A')\). In the case of an isolated partial which formerly was a leading one an additional problem arises as kinks of the opposite sign move to the bends on the straight segments and annihilate kinks in the bend. This annihilation of kinks is in concurrence with the generation of kinks in the apex. As the stress at the apex, which drives the dislocation in the reverse direction, is higher than at any other part of the dislocation the probability of kink formation is enhanced there to overcome the loss of kinks by annihilation at the outer part of the bend. The former trailing partial at the beginning of the relaxation process again moves in the former forward direction. Therefore the mechanism described for the forward motion can be applied.

Finally the problem of curved dislocations in materials with high Peierls energy shall be discussed. As a dislocation lying in a Peierls trough is energetically favoured one should assume that a low stress would not be able to form a curved dislocation. It is, however, well known that if the deforming stress is low (i.e. the temperature is high) most of the dislocations are curved becoming the more straight the higher the applied stress is.

This paradoxical behaviour can be explained by the concept outlined before. The kinks generated on the straight dislocation segments of a dislocation loop which is extending on the glide plane are travelling to the bends and are collected there. If the stress is low, the number of kinks in the equilibrium state is high; if the stress is high, the kinks are more and more forced towards the apex and their number is low because of the annihilation processes. The result therefore is that the portion of straight dislocation segments for a loop of given diameter increases with increasing stress. The intrinsic reason for the formation of curved dislocations is based on the property of the dislocation to be mobile, and that is equivalent to the property of nucleating double kinks. Since these kinks which already had overcome the Peierls hills are always present and their formation energy must not be brought up by the bent dislocation segments, no information on the Peierls energy can be obtained from the curvature of the bends.

Acknowledgements - The author wishes to thank Prof. Dr. H. Alexander and Dipl.-Phys. A. Tönnesen for stimulating discussions on these problems.

References

1/ Gottschalk, H., this conference
2/ Hirth, J.P. and Lothe, J., Theory of Dislocations (McGraw Hill), 1968, Chapt.8-8