

# DISCRETE DISLOCATION CALCULATIONS OF THE STORED ENERGY OF COLD WORK

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**Summary** The stored energy of cold work is calculated for single crystals deformed in plane strain tension and bending. Plastic deformation occurs through dislocation glide. Superposition is used to represent the solution of boundary value problems in terms of the infinite fields for discrete dislocations and image fields that enforce boundary conditions. Constitutive rules are used which account for the effects of 3D dislocation dynamics such as dynamic junction formation. The change in free energy with a change in dislocation positions at constant stress can be explicitly calculated with the line energy contribution accounted for. The extent to which the energy stored in the sample depends on the deformation state is analyzed.

## INTRODUCTION

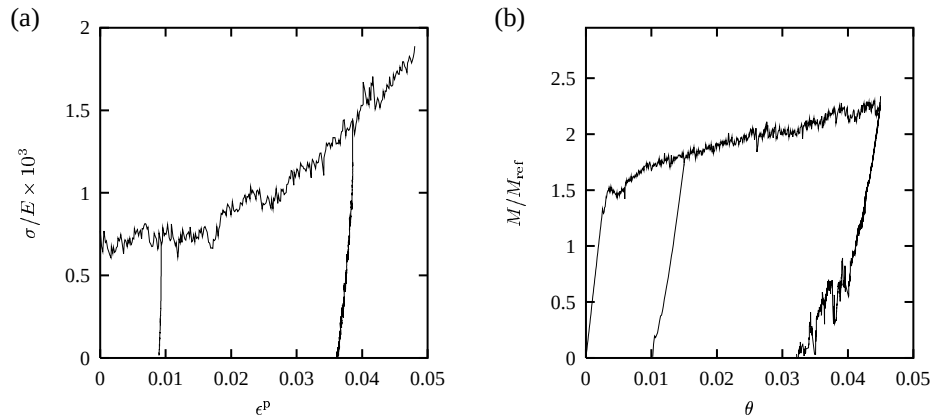
When a material sample is cold-worked, most of the mechanical energy expended is converted into heat and the remainder is stored in the sample, thereby altering its free energy. In single crystals, energy storage is essentially due to dislocations. Here the stored energy due to plastic deformation is calculated as the change in free energy with a change in dislocation positions at constant stress. Such calculations are made feasible by solving boundary value problems where plastic behavior results from the motion and interaction of large numbers of dislocations. These are modeled as linear defects in an isotropic elastic solid and superposition is used to accurately account for the image fields which correct for actual boundary conditions [1]. Dislocation interactions at short range are treated as in [2]. 2D plane strain problems are formulated for the sake of computational efficiency as in [1], but account is taken of 3D dynamic processes such as junction formation and destruction and dynamic source operation. The stored energy calculations are illustrated for two deformation states: tension and bending.

## FORMULATION

Calculations are carried out for a planar fcc  $6\mu\text{m} \times 2\mu\text{m}$  crystal. In tension the calculations of [2] are supplemented by unloading sequences at strain intervals of 0.01. In bending a special numerical procedure is used to assure vanishing of the axial force and unloading sequences are carried at rotation intervals of 0.015. The stored energy rate is equal to the free energy rate, which can be readily calculated using the elastic solution of the boundary value problem. Part of that stored energy is recoverable upon unloading and represents the elastic portion of it. The other portion represents the portion of the plastic work that is not converted into heat but stored in the dislocation structure. The stored energy is calculated both in the unloaded state, as in experiments, and in the loaded state. Initial conditions and material parameters correspond to the crystal labeled B in [2].

## RESULTS

### Loading response



**Figure 1.** Response in (a) tension and (b) bending ( $M_{\text{ref}} = 33.3\mu\text{Nm/m}$ ).

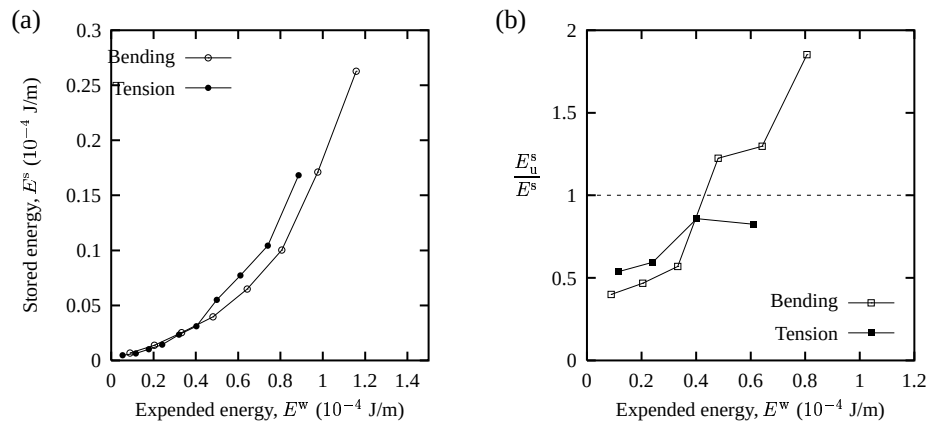
The response in tension shown in Fig. 1(a) exhibits a two-stage hardening as is usually the case for crystals oriented so

that only one slip system is initially activated. The figure also illustrates two unloading sequences from a total strain of 0.01 and 0.04. During the linear stage II hardening a rough cell structure develops so that, upon unloading, reverse yielding occurs while the sample is still in tension. This indicates a strong Bauschinger effect, which almost disappears in the absence of a dislocation structure as detailed elsewhere.

Figure 1(b) shows the moment versus rotation response in bending of the same sample including unloading after  $\theta = 0.015$  and  $\theta = 0.045$ . Here hardening is linear throughout and, after a sufficient amount of bending prior to unloading, reverse yielding is clearly seen while the global moment is still positive. A dislocation structure develops regardless of the density of dynamic junctions. Long arrays of like-signed dislocations are formed on each slip system to accommodate the imposed strain gradient. Those arrays define a density of geometrically necessary dislocations. In [3] it was shown that about 80% of the dislocations are GNDs up to a bending angle  $\theta = 0.06$ . More recent calculations pursued up to  $\theta = 0.12$  clearly demonstrate that the GNDs dominate the global moment-rotation response even at higher angles where the GND density becomes as low as 20% of the total density.

## Stored energy

In order to compare the behavior under the two deformation states (tension and bending) the stored energy under load,  $E^s$ , is plotted in Figure 2(a) against the total work,  $E^w$ , expended in deforming the crystal. For a given supplied  $E^w$  it appears that the rate of energy storage *under load* is independent of the state of deformation. This is remarkable given that the loading response (Fig. 1 above) and the dislocation structure are very different in tension and bending.



**Figure 2.** Energy storage under two deformation states, tension and bending. (a) Stored energy,  $E^s$ , versus expended energy,  $E^w$ . (b) Ratio of stored energy in the unloaded state,  $E_u^s$ , to  $E^s$  versus  $E^w$ .

Upon unloading, however, the rate of energy storage is found to be dependent upon the deformation state. This is best illustrated by considering the stored energy after load removal,  $E_u^s$ , relative to the stored energy under load,  $E^s$ , for a given supplied mechanical energy  $E^w$ . As shown in Fig. 2(b), a significant fraction of the stored energy is released in tension upon unloading. By way of contrast, energy release after unloading in bending only occurs at low values of the bending angle. Depending on the amount of supplied external energy, the energy stored in the unloaded state can be smaller or higher than that of the loaded state.

## CONCLUSIONS

The loading response (flow stress, hardening and unloading) is controlled by the density of statistical dislocations in tension and by the density of GNDs in bending. In bending, however, the build-up of a statistical density strongly affects the magnitude of energy stored in the bent sample after load removal. This suggests important consequences for recrystallization in bending in comparison with tensile loading.

## References

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