Influence of dislocations on a crystal density: Atomistic and continuum modelling

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The density of metals usually decreases with cold work. Zener first explained the origin of this phenomenon in 1942 [4]. Zener connected the change of crystal volume with two facts: the crystal contains some amount of internal stresses and the crystal lattice is "stiffer" for compression than for extension. In the next years, the observation of Zener was confirmed by three methods:

- *experiment* – correlation between dislocation density, stored energy, and volume change suggested that dislocations decrease material density;
- *continuum mechanics analysis* – the second order nonlinear elasticity analysis and the principle of force equilibrium lead to the formula for increase of material volume in a state of self-stresses. According to the Toupin and Rivlin formula [3], every dislocation decreases crystal density;
- *atomistic simulation* – results of atomistic simulations also confirm that crystal density is changed by dislocations, e.g. [2]. An edge dislocation increases volume by 0.25–1.0 $|b|^2$ per unit length of the dislocation line.

However, the above view is inconsistent with results of Bell's experiments [1]. He showed that plastic deformation may contract a crystal. The current theories and available computational results do not explain the results of Bell's experiments. **The results reported in this communication prove that the current view on crystal density changes caused by dislocations is incomplete.**

The analysis explores the Kröners continuum theory of dislocations with the finite element method and, as a second methodology, molecular simulations. The obtained results of continuum and atomistic simulations confirm Bell's results. It is shown that edge dislocations may contract the crystal. Additionally, the origin of the contraction is identified. In the current communication the physical interpretation is proposed to explain why in some cases nucleation of dislocations leads to crystal contraction, while in others leads to dilatation. The obtained results suggest that the general formula of Toupin and Rivlin is incorrect in some cases of self-stressed bodies.

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References

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