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Editorial

Crystal Dislocations: Their Impact on Physical Properties of Crystals

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It is rare to find technical applications involving a material of any crystal structure that is not impacted by dislocations—which affect the material's mechanical properties, interfaces, martensitic phase transformations, crystal growth, and electronic properties, to name a few. In many systems the properties are controlled by the formation of partial dislocations separated by a stacking fault; for example, plastic deformation via dislocation slip and plastic deformation via deformation twinning. In other systems the electronic properties are affected by acceptor or donor states associated with changes of the electronic state of atoms corresponding to the dislocation core of perfect or partial dislocations. Crystal growth often occurs at growth ledges, which can be associated with dislocations. This Special Issue on "Crystal Dislocations: Their Impact on Physical Properties of Crystals" covers a broad range of physical properties involving dislocations and their impact on crystal properties, and contains a mixture of review articles and original contributions.

The influence of dislocations on properties in transition metal oxides was reviewed by Szot et al. [1]. Their review focuses on the important role of dislocations in the insulator-to-metal transition and for redox processes in prototypic binary and ternary oxides (such as TiO_2 and $SrTiO_3$) examined using transition electron microscopy (TEM) and scanning probe microscopy (SPM) techniques combined with classical etch pits methods. Since dislocations play a critical role in the plastic deformation of materials, several contributions deal with a detailed understanding of dislocations and their influence on the mechanical properties of materials. The plastic deformation in magnesium oxide crystals, MgO, being an archetypal ionic ceramic with refractory properties of interest in several fields of applications such as ceramic materials fabrication, nanoscale engineering, and earth sciences, was reviewed by Amodeo et al. [2]. Their review describes how a combined approach of macro-mechanical tests, multi-scale modeling, nano-mechanical tests, and high-pressure experiments and simulations have helped to improve the understanding of the mechanical behavior of MgO and elementary dislocation-based processes. The structure of the basal edge dislocations in ZnO was examined by Nakamura et al. [3]. The dislocation core structure was observed using scanning transmission electron microscopy (STEM) at atomic resolution, and it was found that a basal edge dislocation dissociated into $1/3\langle 1\bar{1}00\rangle$ and $1/3\langle 10\bar{1}0\rangle$ partial dislocations on the (0001) plane, separated by a stacking fault with a stacking fault energy of 0.14 J/m^2. The importance of stoichiometry on the mechanical properties of $SrTiO_3$ was also examined by Nakamura et al. [4] through studies of the room-temperature plasticity of strontium titanate crystals grown from source materials having varying Sr/Ti ratios. It was found that the flow stresses of $SrTiO_3$ crystals grown from a powder with a Sr/Ti ratio of 1.04 were almost independent of the strain rate which, in turn, is believed to be due to the high dislocation mobility in such crystals.

Several contributions examined the impact of dislocations on the mechanical properties in metallic systems. Keshavarz et al. [5] developed a framework to obtain the flow stress of nickel-based super alloys as a function of $\gamma - \gamma'$ morphology, as the yield strength is a major factor in the design of such alloys. In order to obtain the flow stress, non-Schmid crystal plasticity constitutive models at two length scales were employed and bridged through a homogenized multi-scale framework. The importance of stacking faults in $Al7075$ formed through precipitate and dislocation interactions was examined by Li et al. [6] using high-resolution electron microscopy. Stacking faults due to Frank partial dislocations were found following deformation using low strain and strain-rates, and extrinsic stacking faults were found to be surrounded by dislocations and precipitates whereas an intrinsic stacking fault was found between two Guinier-Preston II (GP II) zones when the distance of the two GP II zones was 2 nm. The anisotropic plastic behavior in two metallic systems was examined; Wei et al. [7] reported on the anisotropic plastic behavior in aluminum single crystals by crystal plasticity finite element methods and Bian et al. [8] examined the anisotropic plastic deformation in the compression of single crystalline copper nanoparticles. The dislocation-dopant ions interaction in ionic crystals by strain-rate cycling tests with the Blaha effect measurement was reviewed by Kohzuki [9]. The strain-rate cycling test during Blaha effect measurement has successively provided information on the dislocation motion breaking away from the strain fields around dopant ions with the help of thermal activation, and seems to separate the contributions arising from the interaction between dislocation and the point defects and those from dislocations themselves during the plastic deformation of ionic crystals.

The importance of dislocations on phase transformation was examined by Hu et al. [10], in which they studied phase transformation and hydrogen storage properties of an $La_{7.0}Mg_{75.5}Ni_{17.5}$ hydrogen storage alloy. Differential thermal analysis showed that the initial hydrogen desorption temperature of its hydride was 531 K and, compared to Mg and Mg_2Ni, $La_{7.0}Mg_{75.5}Ni_{17.5}$ was found to be a promising hydrogen storage material that demonstrates fast adsorption/desorption kinetics as a result of the formation of an $La - H$ compound. Since some phase transformations, e.g., martensitic phase transformations, involve the motion of interface dislocations, it is important to understand the properties of such dislocations. In addition, the details of partial dislocation making up perfect dislocations are important for both the plastic deformation of materials via the dislocation motion of dissociated perfect dislocations and deformation twinning involving the motion of partial dislocations. One way of producing such dislocations is to fuse crystals with surfaces having controlled crystallographic planes to make low-angle grain boundaries for subsequent characterization. Tochigi et al. [11] reviewed the dislocation structures in $\alpha - Al_2O_3$, obtained using systematically fabricated alumina bi-crystals with low-angle grain boundaries and characterized using transmission electron microscopy (TEM). Wang et al. [12] examined the interface effects on screw dislocations in Al/TiC hetero-structures, which was used as a model interface to study the unstable stacking fault energies and dislocation properties of interfaces. It was found that the mismatch of lattice constants and shear modulus at the interface resulted in changes of the stacking fault. However, in many cases it is desirable to eliminate interface dislocations altogether, and Montalenti et al. [13] reviewed dislocation-free $SiGe/Si$ hetero-structures grown on deeply patterned $Si(001)$, providing possibilities of growing micron-sized Ge crystals largely free of thermal stress and hosting dislocations only in a small fraction of their volume. They also analyzed the role played by the shape of the pre-patterned substrate in directly influencing the dislocation distribution.

Finally, the effect of dislocations on peak broadening anisotropy and the contrast factor in metal alloys characterization using X-ray diffraction was reviewed by Simm [14]. Peak broadening anisotropy, in which the broadening of a diffraction peak does not change smoothly with d-spacing, is an important aspect of diffraction peak profile analysis (DPPA) and is a valuable method to understand the microstructure and defects present in the material examined. There are numerous approaches to deal with this anisotropy in metal alloys, which can be used to gain information about the dislocation types present in a sample and the amount of planar faults. However, there are problems in determining which method to use and the potential errors that can result, in particular for hexagonal close-packed (*hcp*) alloys. There is, however, a distinct advantage of broadening anisotropy in that it provides a unique and potentially valuable way to develop crystal plasticity and work-hardening models.

The present Special Issue on "Crystal Dislocations: Their Impact on Physical Properties of Crystals" can be considered as a status report reviewing the progress that has been achieved over the past several years in several subject areas affected by crystal dislocations.

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