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Editorial

Crystal Dislocations

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Received: 28 December 2015; Accepted: 4 January 2016; Published: 6 January 2016.

Abstract: Crystal dislocations were invisible until the mid-20th century although their presence had been inferred; the atomic and molecular scale dimensions had prevented earlier discovery. Now they are normally known to be just about everywhere, for example, in the softest molecularly-bonded crystals as well as within the hardest covalently-bonded diamonds. The advent of advanced techniques of atomic-scale probing have facilitated modern observations of dislocations in every crystal structure-type, particularly by x-ray diffraction topography and transmission electron microscopy. The present *Special Issue* provides a flavor of their ubiquitous presences, their characterizations and, especially, their influence on mechanical and electrical properties.

Keywords: dislocations; crystals; polycrystals; nanopolycrystals; x-ray topography; transmission electron microscopy; optical microscopy; crystal growth; crystal strength properties; electrical properties

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1. Introduction

Early interest in dislocations sprang from research investigations into conditions of crystal growth and on subsequent permanent (or plastic) crystal deformation properties, in the latter case, particularly relating to crystal strength and ductility. An important industrial focus on defects in electronic crystals at micro-scale dimensions has led to much ongoing research activity.

Cottrell in 1953 produced a seminal book on dislocations and strength properties based on his teaching at Birmingham [1]. An early conference on dislocation observations, mostly, in metals was held in 1961 [2]. Emphasis was given to observations made via optical and electron microscopy, x-ray diffraction topography, and field ion microscopy. Among a number of subsequent dislocation treatises with broader coverage are books by Nabarro [3] and by Hirth and Lothe [4]. A frequently referenced book is by Hull and Bacon [5]. Nabarro initiated a comprehensive series of *Dislocations in Solids* volumes, latterly co-edited, first with Duesbury, then with Hirth [6], and later by Hirth, then ending with Hirth and Kubin [7]. In all, ninety-six chapters were produced over the period from 1980 until 2010 by many experts. The early volumes 1 to 3 established the elastic theory, lattice relationship and movement properties. Figure 1 shows a schematic view of an edge dislocation with central core and flexible line orientation to circumvent obstacles to migration [8].

2. Crystal Growth and Dislocation Structures

Frank saw first the important advantage in crystal growth of a screw dislocation with displacement (Burgers) vector, b, parallel to line axis, ℓ, and thus providing a consequent never-ending crystal step for atomic attachment [9]. Burton described with Cabrera and Frank the beneficial nature of the trailing spiral ledge [10]. Updated commentary of the crystal growth work by Frank and colleagues and on other work extending until recent time has been given by Woodruff

[11]. Figure 2 is a transmission x-ray topograph of a cm-size α-Al_2O_3 (sapphire) crystal slice from a larger boule grown by a chemical vapor decomposition technique [12]. The just-visible very finely resolved lines are individual dislocations. Three 'blackened' bunches are shown to emanate from individual points across a recognizable upper boundary trace established when the crystal growth had been temporarily halted. Edge type dislocations with b perpendicular to ℓ, as in the front face of Fig. 1, penetrate growth interfaces also, presumably, to incorporate impurities and solutes. Other aspects of dislocation arrangements have been reported for zinc, nickel and (photovoltaic) silicon crystals [8].

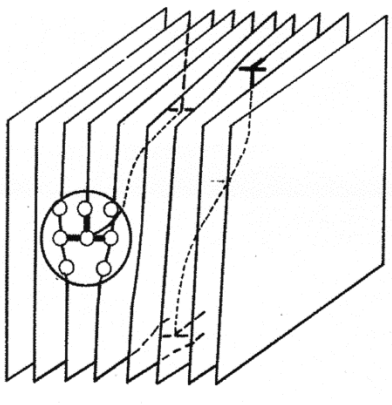

Figure 1. Schematic dislocation picture.

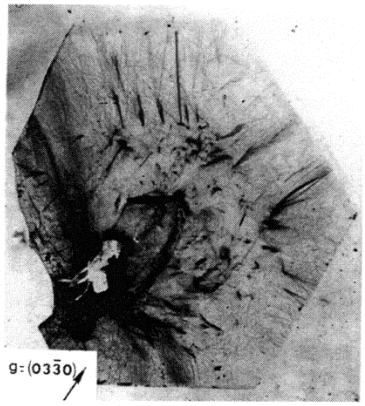

Figure 2. Dislocations in α-Al_2O_3 crystal.

3. Crystal, Polycrystal, Nanopolycrystal Deformations

Dislocations move relatively easy in metal crystals or polycrystals, and less so in ionic, covalent and molecular crystals. One might note indication in Fig. 1 of mutual impediment indicated *via* potential dislocation intersections, otherwise there are lattice/solute interactions to be contended with as indicated in Fig. 3. In the figure, the dislocations are denoted as rightside-up or inverted T's and various solute are represented by the black dots, either residing individually, or dislocation-associated in three cases: (i) at individual dislocations, or (ii) on the left side as segregated at dislocations arranged in a vertical subgrain boundary, or (iii) to greater extent, within a (crystal) grain boundary region between adjacent crystals of different lattice orientations. The dotted lines represent 'slip' of the dislocations across the subgrain boundary structure and locally concentrated in the grain boundary region where the direction-dependent strains must necessarily be accommodated.

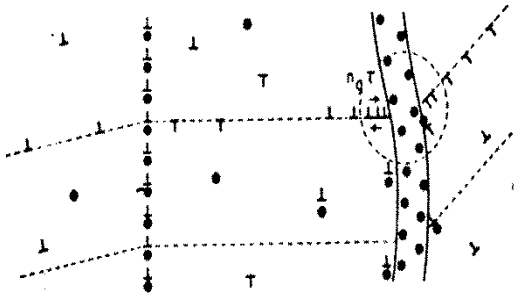

Figure 3. Polycrystal dislocation slip.

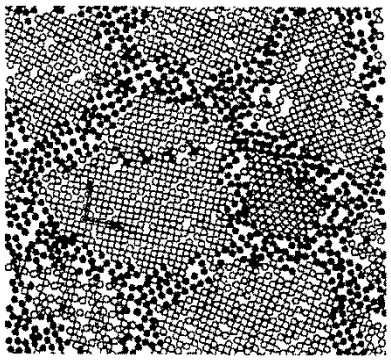

Figure 4. Nanopolycrystal structure.

The polycrystal strength dependence on reciprocal square root of grain size was first reported in independent investigations of the strength properties of steel materials by Hall [13] and Petch [14] and then the same type of grain size dependence was shown later to apply quite generally to the complete stress-strain behaviors of mild steel and to a wider number of metals [15]. An updated review has been presented [16]. An analogous relationship to the crack size dependence of the fracture mechanics properties of metals and related materials has been established [17].

Considerable research interest is currently being devoted to materials nanotechnology in three research areas: (1) nano-indentation hardness testing; (2) mechanical testing of specimens with nano-scale structures; and (3) testing material specimens of physical nano-scale dimensions. A review has been reported on crystal/polycrystal nanoindentation hardness testing [18]. Figure 4 is an atomic scale simulation of the deformation structure within a nickel crystal [19]. A treatise on the structure and properties of nano-scale metals has been edited by Faester, Hansen, Huang, Juul Jensen and Ralph [20]. Relating to Fig. 3, Hirouchi and Shibutani have reported on slip transmission across special Σ3 crystal grain boundaries in very small copper micro-pillars [21].

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