ABSTRACT: Structural models, and geometric criteria for 'special' grain boundary and triple junction properties are presented and assessed on the basis of experimental studies of energetic, kinetic, physical, chemical, and mechanical phenomena; the applicability of these criteria are shown to be due to their importance in defining intercrystalline dislocation structures. Methods of controlling the distribution, quantity and structure of grain boundaries in polycrystalline materials are also presented. Several of the unusual properties exhibited by nanocrystalline materials are shown to be simply a manifestation of an enhanced intercrystalline volume fraction consisting of distinct grain boundary and triple line disclination structures.

1. Geometric Characterization of Grain Boundaries

Kronberg and Wilson [1] first indicated the importance of the concept of a coincidence site lattice (CSL), whereby at certain crystallographic misorientations a 3-dimensional lattice could be constructed with lattice points common to both crystals. The CSL is thus considered the smallest common sublattice of the adjoining grains [2]. The volume ratio of the unit cell of the CSL to that of the crystal is described by the parameter \( \Sigma \) [2], which can also be considered the reciprocal density of coincidence sites [1]. All grain boundaries can be represented by an appropriate CSL description if \( \Sigma \) is allowed to approach infinite values [3]. As will be shown later, special properties of interfaces described by low-\( \Sigma \) CSL relationships have been observed in numerous studies, the earliest of which being the mobility studies of Aust and Rutter [4].

Ranganathan [5] first presented a general procedure for obtaining CSL relationships about general rotation axes. When crystallographically distinct rotations (ie. not symmetry related) lead to the same value of \( \Sigma \), the corresponding CSL's are distinguished by letter designations (a, b, c, etc.) in order of increasing disorientation angles [6]. Mykura [6] has provided a comprehensive list of CSL orientation relationships for \( \Sigma = 1 \) to 101e. Although all grain boundaries can be represented by exact CSL relationships, \( \Sigma \) may
achieve very high values of questionable physical significance. Small angular deviations from low $\Sigma$ CSL relationships can be described as being accommodated by translations of one lattice relative to the other, conserving the periodicity of the exact CSL [2]. These translations result in a network of "secondary grain boundary dislocations" (SGBD's) which conserve the periodicity of the CSL [7]. The Burgers vectors of these dislocations are described by the DSC (Displacement Shift Complete) lattice, which can be considered the coarsest lattice containing the two adjoining crystals as sublattices [2]. The DSC lattice is thus only dependent on the misorientation of the two lattices, and can be considered the reciprocal lattice of the CSL with a unit cell proportional to $\Sigma^{-1}$ [2].

With low angle grain boundaries ($\Sigma = 1$), the CSL and DSC lattices are coincident with the adjoining crystal lattices, and the grain boundaries can be described through lattice dislocations accommodating the deviations from ideal crystal coincidence, i.e. the single crystal [8]. For other CSL related interfaces (i.e. $\Sigma > 1$), the SGBD networks are described by the basis matrix of the DSC lattice [2]. The existence of SGBD networks at CSL related grain boundaries has been experimentally verified by TEM in numerous studies [e.g. 9].

The various criteria for the maximum allowable angular deviation from exact CSL's are largely derived from the low angle approximation of the Read-Shockley relation [8], $\theta = b/d$ where $\theta$ is the misorientation angle, $b$ is the magnitude of the Burgers vector of grain boundary dislocations, and $d$ is the dislocation spacing. Deschamps et al [10] considered a dislocation spacing ($d$) proportional to a mean edge ($p$) of the CSL lattice [2], where $d = p \propto \Sigma^{1/3}$ and Burgers vector magnitude ($b$) varying on average as the mean edge of the DSC lattice [2], such that $b \propto \Sigma^{-1/3}$. However, as shown by Grimmer et al [2], two of the three Burgers vectors described by the DSC lattice vary as $\Sigma^{-1/2}$; the third is independent of $\Sigma$ and varies only as the interplanar spacing along the rotation axis. Thus the only variation of $b$ with $\Sigma$ would be of the type $\Sigma^{-1/2}$. By considering $d \propto \Sigma^{1/3}$, $b \propto \Sigma^{-1/2}$ and an upper angular deviation limit of $15^\circ$ for low angle boundaries (i.e., $\Sigma 1$), the following geometric criterion is obtained [11]: $\Delta \theta \leq 15^\circ \Sigma^{-5/6}$.

Figure 1 shows the maximum angular deviation ($\Delta \theta$) from specific CSL's (ie. $\Sigma$) at which intrinsic grain boundary dislocations (IGBD's) i.e. primary dislocations for $\Sigma = 1$, secondary grain boundary dislocations (SGBD) for $\Sigma \geq 3$, have been observed by TEM. Also shown in Fig. 1 are the various criteria proposed for the angular deviation limit of the CSL. As seen in this figure, resolvable IGBD's are identified with interfaces lying well within the structural limits imposed by both the commonly applied criterion of Brandon [15] (ie. $\Delta \theta \leq 15^\circ \Sigma^{-1/2}$), and the proposed criterion of Deschamps et al [10] (ie. $\Delta \theta \leq 15^\circ \Sigma^{-2/3}$); also the maximum deviation angles tend to extend beyond the more restrictive criterion proposed by Ishida and McLean [16] (ie. $\Delta \theta \leq 15^\circ \Sigma^{-1}$). However, the geometric criterion $\theta \leq 15^\circ \Sigma^{-5/6}$ is shown to be the most consistent with the experimental observations of discrete IGBD's summarized in Fig. 1.

In evaluating the applicability of the CSL/DSC model to interfacial properties, it is also important to consider an upper limit for the $\Sigma$ criterion beyond which special properties would not be expected. As seen in Fig. 1, discrete IGBD's have been identified with CSL's having very high $\Sigma$ values (ie. $\Sigma > 49$), indicating that some structural order can exist at these interfaces. However, on the basis of experimental studies concerning