MOVEMENT OF COINCIDENCE GRAIN BOUNDARIES WITH SIGMA = 7, 13, 19, $\cdots, 49, \cdots, 91, \cdots$: FROM ISOTROPY TO ANISOTROPY

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1. Isotropy

Isotropy means having the same properties in all directions (1856). The word is derived from the Greek, *isos* (equal) and *tropos* (way). The exact definitions depend on the field in which this concept is used. The opposite of isotropy is anisotropy. The term isotropy is associated with geometry and the concept of direction, while the term of homogeneity is associated with the concept of density. Simple chemical reaction and removal of a substrate by an acid or a solvent or is often close to isotropic. The kinetic theory of gases is also an example of description of the isotropic medium, cf. [1]. In Statistical Physics, for the system of N particles, the two-particle distribution function $n_2 = n_2(\boldsymbol{r}_1, \boldsymbol{r}_2)$ is defined as $n_2(\boldsymbol{r}_1, \boldsymbol{r}_2) = N(N-1)P_2(\boldsymbol{r}_1, \boldsymbol{r}_2)$, where $P_2(\boldsymbol{r}_1, \boldsymbol{r}_2)$ is the probability density to find particle nr 1 at $\boldsymbol{r}_1$ and nr 2 at $\boldsymbol{r}_2$. For isotropic system $n_2(\boldsymbol{r}_1, \boldsymbol{r}_2) = n_2(r_{12})$, cf. [2]. In Chemistry, the electron clouds described by s-orbitals are isotropic, and by other orbitals - anisotropic, cf. [3]. In Economics and Geography, an isotropic region is a region that has the same properties everywhere. The Big Bang theory of the evolution of the observable universe assumes that space is isotropic. It also assumes that space is homogeneous. These two assumptions are known as the Cosmological Principle, [4, 5].

Amorphous substances are isotropic, although they do not have to be homogeneous. Polycrystalline bodies may also be isotropic. If the individual crystallites are oriented completely at random, a large enough volume of polycrystalline material will be approximately isotropic. In hydrodynamics, we observe with the increasing velocity the passage from the laminar flow (anisotropic) to turbulent (isotropic) flow, cf. [6].

2. Isotropy and anisotropy in geometry and mechanics

Carl F. Gauss proved that the highest average density in close-packing of equal spheres is equal to $\pi/(3\sqrt{2}) \simeq 0.74048$ in 3D, and $\pi/(2\sqrt{3}) \simeq 0.9069$ in 2D. The Kepler conjecture, recently proved states that this is the highest density that can be achieved by any arrangement of spheres, either regular or irregular, cf. [7–9].

A hexagonal 2D crystal is anisotropic and has three symmetry axes. A deformation in the plane is determined by only two moduli of elasticity, as for an isotropic body, cf. [10]. A symmetric tensor of rank two, such as the termal conductivity or the termal expansion tensors have only one component, again as in isotropic medium.

Conversely, an isotropic medium subject to stress acquires anisotropic properties, behaves like a crystal and exhibits the birefringence, [11]. Similarly, the isotropic suspension of magnetic particles (in micrometer or nanometer scale spheres) sitributed randomly becomes in the magnetic field an anisotropic solid, [12].

3. Coincidence site lattice

A grain boundary is the interface between two kinds of grains, or crystallites, in a polycrystalline material. The boundary consists of structural units which in the 2-D system depend on the misorientation of the two neighbouring grains. The misorietation angle is given by

$$\alpha = \arccos \frac{d^2 + n^2 - m^2}{2\,d\,n} \quad \text{where} \quad d^2 = m^2 + n^2 + m\,n$$

and m, n are integers. The types of structural unit are described by the concept of the coincidence site lattice (CSL), in which repeated units are formed from points at which the two misoriented lattices happen to coincide.

The degree of fit (Σ) between the lattices of the two grains is described by the reciprocal of the ratio of coincidence sites to the total number of sites

$$\Sigma \equiv \frac{\text{surface of the CSL unit cell}}{\text{surface of the lattice unit cell}}$$

It is possible to draw the lattice for the 2 grains and count the number of atoms that are shared (coincidence sites), and the total number of atoms on the boundary (total number of site). For example, when $\Sigma = 7$ there will be one atom each 7 that will be shared between the two lattices. The misorientation angle $\alpha = 19.1066^{\mathrm{o}}$ for $\Sigma = 7$, as in this case $m = 1, n = 2, d = \sqrt{7}$.

4. From isotropy to anisotropy

We are considering a 2-D system of point particles subject to periodic boundary conditions. To ensure uniform homogeneous density of the initial arrangement, we distribute the particles on the honey-comb lattice. In each cell of this lattice we randomly put 7 particles . In such a way the isotropic initial system is created.

Next, all the particles of the system are subjected to the Centroidal Voronoi iterations. One of the 7 particles in each honey-comb cell after a few iterations approaches to the very center of the cell. In this way, a coincidence point appears in the center of each honey-comb cell. After just a few iterations, the system begins to crystallize in two phases of different directions. During the further crystallization convexities and concavities of the grain boundaries are reduced and the grain boundaries straighten.

Thus, the consecutive iterations result in increasing the anisotropy by disappearing some pentagons-heptagons (5-7) pairs. As a result, the percentage of hexagons increases and in consequence the anisotropy is growing. The same procesure could be done for $\Sigma = 13, 19, \cdots$ and in general $\Sigma = 6\,k + 1,\ k = 4, 5, 6, \cdots$. After each iteration we examine the number of hexagons created. The increase in their number is a measure of the departure from isotropy. Finally, we observe the creation of a bicrystal formed by grains ofr only two kinds. Two phases are separated by the boundary of 5-7-pairs. It is important that contrary to the widespread opinion that the 5-7 pairs are symmetric, these 5-7 pairs do not lie on the boundaries in a symmetrical manner.

If other (not coincident) integer numbers are put in the honey-comb lattice cells, we get polycrystals. But, if $\Sigma = 49 = 7 \times 7$ and $\Sigma = 91 = 7 \times 13$ it is possible to build up interesting tricrystals.

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