Complexions: A Revolutionary Taxonomy for Grain Boundaries

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Taxonomy: Classification, especially in relation to its general laws or principles. (OED)

The world has far too many things in it to treat them all individually. One way we make progress is through taxonomy. We group things so as to be able to discuss them usefully and understand them. The best-known taxonomy is that of living things: we group them as mammals, reptiles, grasses, trees. We group crystals based on their symmetry: cubic, hexagonal, orthorhombic.

Grain boundaries remain one of the main outstanding problems in materials science. We understand crystals rather well, but we do not have a good science of grain boundaries yet. It would help to have a taxonomy of grain boundaries.

Until recently, what seemed to be the most promising taxonomy for grain boundaries was based on a set of ideas leading to a distinction between "special boundaries" and "general boundaries." The simplest special boundary is the coherent twin boundary. However, more generally, special boundaries are identified by the relative orientations of the two grains that meet at the boundary. Such special boundaries are called coincident site lattice (CSL) boundaries.

Two groups have recently presented work that implies that we should abandon the CSL approach and turn to a new taxonomy. The first work is from Greg Rohrer's group at Carnegie-Mellon. They have done detailed work with EBSD and found that, in general, CSL analysis does not help understand the huge data sets that they have obtained on grain boundary statistics[1]. This suggests that the CSL taxonomy is not as useful as had been supposed.

The second piece of work comes from the group of my colleague, Martin Harmer, here at Lehigh. Through careful studies by aberration-corrected TEM and other techniques, they have found that they can classify grain boundaries in a new way[2]. Each "family" of grain boundaries is found to have a unifying set of properties (even though the details of the boundary structure may be very different—just as cats and dogs are different, though both are mammals, and have unifying characteristics). They call these families: "complexions": see figure 1. Moreover, they have developed phase diagrams to show which complexions occur at which temperatures and doping (or impurity) levels, see figure 2.

Phase diagrams for grain boundaries—that seems like real progress to me. ■

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References:

1. David M. Saylor, Bassem S. El Dasher, Anthony D. Rollett and Gregory S. Rohrer *Distribution of grain boundaries in aluminum as a function of five macroscopic parameters,* Acta Materialia **52** (2004) 3649-3655
2. Shen J. Dillon, Ming Tang, W. Craig Carter and Martin P. Harmer, *Complexion: A new concept for kinetic engineering in materials science,* Acta Materialia **55** (2007) 6208-6218

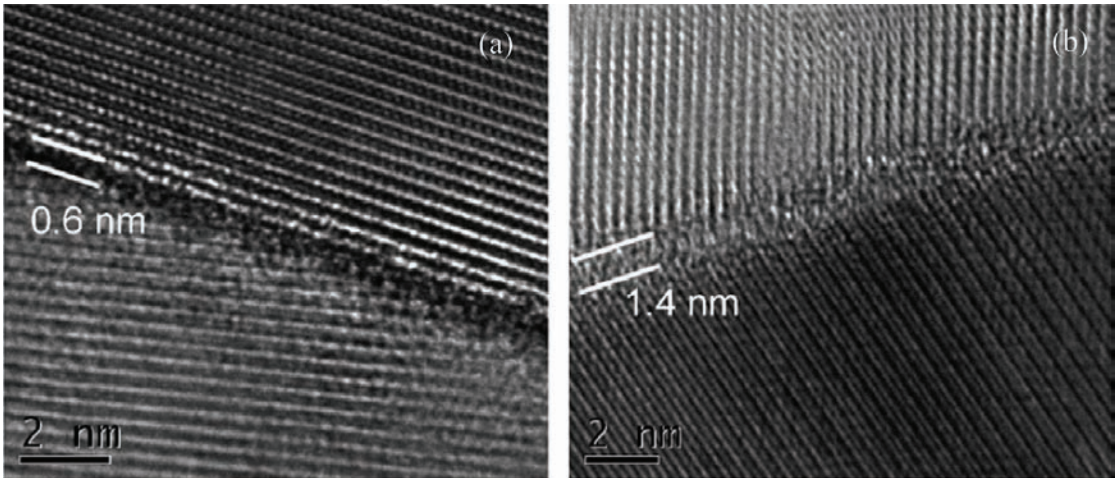

Figure 1: Examples of two different complexions in alumina doped with silica. The grain boundary phases can be distinctly different depending on the dopant concentration and the sintering/annealing temperature. (a) is an example of complexion IV while (b) is an example of complexion V. (See reference 2)

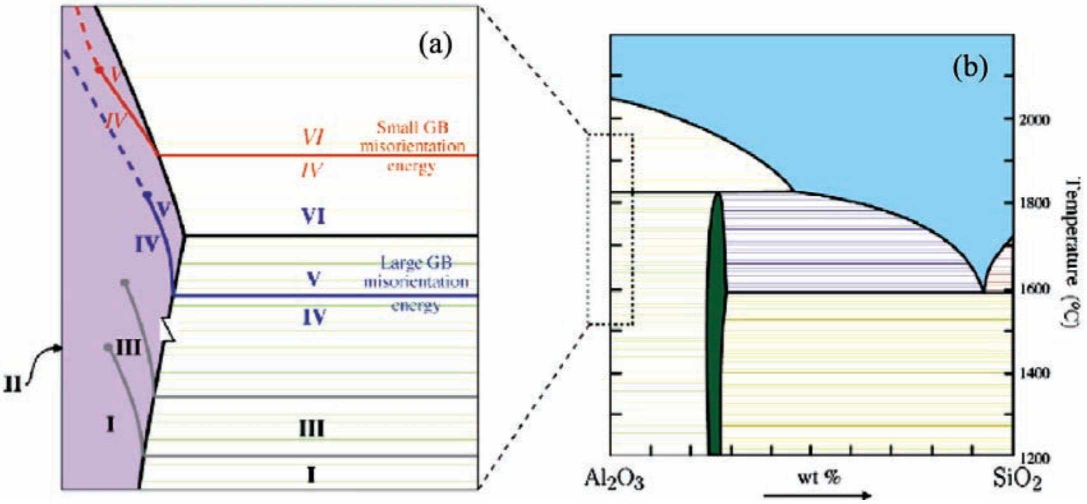

Figure 2:(a) Schematic drawing of a complexion diagram for the binary eutectic system, Al_2O_3–SiO_2, whose bulk phase diagram is shown in (b), with labels denoting the stable regions of different complexions. The complexions are named with roman numerals: I, II, III, etc. The grain boundaries take the form of different complexions depending on the temperature and composition of the material. Diagram (a) gives a tentative and approximate representation of which complexion is stable under which conditions. (See reference 2)

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