**Statements on the transition from high to low mobility based on temperature**

Starting paper: Miao *et al*. “*In Situ* Synchrotron Investigaion of Grain Growth Behavior of Nano-grained UO2”, *Scripta Materialia* 131 (2017) 29-32

* Each citation (starting with Olmsted *et al*.) is highlighted with the associated color in the original text (e.g. in Miao *et al*., “…types of grain boundaries[23]…” has the [23] highlighted green, and the associated paper is Olmsted *et al*., highlighted green)
* If a paper is not currently accessible, the citation is blacked out (black background).

**Miao *et al.*:** Each type of grain boundary has a [characteristic temperature](https://www.sciencedirect.com/topics/physics-and-astronomy/temperature-characteristics), Tc, at which the grain boundaries transition from low-mobility to high-mobility. The characteristic temperatures can vary by a considerable amount due to the variation in activation energy of different types of grain boundaries[[23]](https://www.sciencedirect.com/science/article/pii/S135964621630625X" \l "bb0115). Namely, at a specific temperature, T, only those grain boundaries with Tc < T have high-mobility and therefore contribute effectively to grain growth.

**Miao *et al.* 🡪Olmsted *et al.*:** two important temperature-dependent phenomena are non-activated boundary motion and the boundary roughening transition, which we discussed earlier for a few individual boundaries [[25]](https://www.sciencedirect.com/science/article/pii/S1359645409002316" \l "bib25).

Both faceted and unfaceted boundaries are observed to undergo a transition from a smooth configuration to a rough configuration as temperature increases [[37]](https://www.sciencedirect.com/science/article/pii/S1359645409002316" \l "bib37), [[38]](https://www.sciencedirect.com/science/article/pii/S1359645409002316" \l "bib38). We previously described the characteristics of the ideal roughening transition for activated boundary motion [[25]](https://www.sciencedirect.com/science/article/pii/S1359645409002316#bib25). At low temperatures, the boundary is smooth; boundary mobility is low and decreases as the driving force tends to zero; and boundary motion is stepwise in units consistent with the atomic repeat distance. At the roughening temperature Tr, there is a jump in mobility. Above Tr, the boundary is rough; boundary mobility is high and constant with driving force; and boundary motion is continuous. We note that among the boundaries we have studied, there are many exceptions to this “ideal” roughening behavior, including the non-activated motion described above.

**Miao *et al.* 🡪Olmsted *et al.* 🡪 Olmsted *et al.*:** It is well known that surfaces and interfaces, including grain boundaries, undergo a roughening transition because of the competition between energy, which favors a smooth boundary, and entropy, which favors a rough one.

In this paper we show that, even for non-faceting boundaries, mobility is very different above and below the interface roughening transition. And since we also show that the roughening temperature itself can vary substantially with grain boundary crystallography, it is clear that the effect of roughness on grain boundary mobility requires more attention than it has received.

Interestingly, at high driving force, the mobility of boundary I at 800 K appears to become consistent with the mobility predicted by the activation barrier derived from the higher temperature data. This suggests that the mechanism of boundary motion has become indistinguishable from that of the rough boundaries. We conjecture that the 800 K boundary has become “dynamically” roughened at high driving force.

It appears that there is a large discontinuity in mobility between smooth and rough boundaries that is mitigated at high driving forces.

**Miao *et al.* 🡪Olmsted *et al.* 🡪Yoon and Cho:** Usually, the defaceting transition is thus a manifestation of the grain boundary roughening transition.

In many metals and oxides [15, 16, 17, 18, 19, 20, 21, 22], abnormal and normal grain growth behaviors were observed to be correlated with grain boundary roughening.

Aust [29, 64] and Gleiter [65] made apparently the first suggestions that grain boundaries underwent phase transition, based on their analysis of grain growth kinetics and triple junction equilibria in Pb and its alloy. In 1970, Hart [66] also made the same suggestion and performed a thermodynamic analysis of this transition assuming it to be a first order transition[67].

While surface roughening occurs at temperatures close to the bulk melting point Tm, the grain boundary roughening can occur at temperatures below Tm.

It now appears that the grain boundaries in all metals examined so far undergo roughening transitions at temperatures above about 0.7 Tm. The twin boundaries and some grain boundaries may remain singular even at the melting point.

If a grain boundary is rough, its structure and properties will be nearly isotropic with respect to both the misorientation angle between the grains and the boundary plane.

In metals and oxides, it was shown that the grain growth behavior was closely correlated to the grain boundary roughening transition [15, 16, 21, 22, 91, 92, 93, 94, 95, 96, 97].

It is expected that in such a case, the properties are expected to vary from the singular to rough boundaries, and the migration of the intersecting grain boundaries including that of the triple junction will critically depend on temperature because of the boundary transformations.

**Miao *et al.* 🡪Olmsted *et al.* 🡪Yoon and Cho 🡪 Lee *et al.*:** In the carburized specimens, normal grain growth occurred at temperatures above 0.7Tm (936 °C) and AGG occurred below 0.7Tm. In the specimens annealed under vacuum, AGG occurred at all temperatures between 0.55and 0.95Tm. Except during the early incubation period, all or a fraction of the grain boundaries in the specimens showing AGG were faceted. In contrast, all of the grain boundaries in the specimens showing normal grain growth were defaceted, with smoothly curved or nearly straight grain boundaries. Thus, a correlation was found between the grain boundary faceting and AGG.

Even after prolonged annealing treatments, only a fraction of the boundaries can be faceted, apparently because the transformation temperatures vary among the grain boundaries.

The results of these double annealing experiments thus confirm that the grain growth mode, either normal or abnormal, for the carburized specimens depends on the annealing temperature, as illustrated in Figure 1.

The present study shows that the general grain boundaries in a polycrystalline material with random misorientations between the grains and random average boundary orientation (inclination angle) also undergo faceting transformation with temperature change as well as with additives.

Only in the systems with textures did the computer simulations predict AGG if the grain boundaries were anisotropic [71,72]. It, thus, appears that without any texture, the anisotropy of the grain boundary energy itself does not cause AGG. 🡨 *Not directly related to what I’m currently studying, but important nonetheless.*

**Miao *et al.* 🡪Olmsted *et al.* 🡪Yoon and Cho 🡪 Koo and Yoon:** *Nothing particularly stands out here. AGG is correlated with the faceting of grains, and normal grain growth is associated with grain boundary roughening.*

**Miao *et al.* 🡪Olmsted *et al.* 🡪Yoon and Cho 🡪 Park and Yoon:** However, when the MgO concentration is sufficiently high to cause the step free energy to become zero, all the grains can grow continuously and, hence, normal growth occurs. Therefore, the transition from AGG to normal growth with increasing MgO concentration will be continuous as the number of the rapidly growing grains increases. A similar transition from AGG to normal growth is expected with increasing temperature, as proposed earlier. [24] *Note that this source is title “The Step Growth Hypothesis for AGG,” thus I do not expect it to specifically relate to the temperature dependence of high- vs low-temperature mobilities.*

**Miao *et al.* 🡪Olmsted *et al.* 🡪Yoon and Cho 🡪 Park *et al*.:** A surface roughening transition occurs with either temperature increase or composition change when the step free energy becomes 0.

*This paper mainly talks about composition effects, not temperature effects (only one temperature examined)*.

**Miao *et al.* 🡪Olmsted *et al.* 🡪Yoon and Cho 🡪 Lee, Chung, and Kang:** *Nothing of particular interest is said in this paper relevant to the current topic. Only one (annealing) temperature was used.*

**Miao *et al.* 🡪Olmsted *et al.* 🡪Yoon and Cho 🡪 Cho *et al.***: (Note that the publication can be found [here](https://ceramics.onlinelibrary.wiley.com/doi/pdf/10.1111/j.1551-2916.2004.00119.x).) *Still mainly concerned with concentration effects, though there are three sintering temperatures examined. Too many variables changed between the different microstructures however, so there is not a clear relationship between high- vs low-mobility and temperature.*

**Miao *et al.* 🡪Olmsted *et al.* 🡪Yoon and Cho 🡪 Choi and Yoon:** In one experimental series, a specimen was first heat-treated at 1 100°C for 60 min to obtain an AGG structure with a few grains as large as 400mm as shown in Figs. 2(c)and 3. When this specimen was heat-treated again at 1 300°C, the fine matrix grains coarsened but the largest grains did not grow abnormally as shown in Fig. 8. The grain size distribution thus appeared to approach that of normal growth, which is expected to occur at 1 300°C. This result shows that even the abnormally large grains produced at 1 100°C did not continue to grow abnormally when the growth mechanism was changed with the rough grain boundaries at 1 300°C.

In another step heat-treatment series, the specimens were first heat-treated at 1 300°C for different periods to obtain grains of various average sizes by normal growth. When these were heat-treated again at 1 100°C AGG occurred if the initial average grain size obtained by normal growth at 1 300°C was relatively fine. These results confirmed that the growth behavior could be readily varied by temperature change.

Thus, with increasing temperature the grain growth behavior will resemble normal growth and will be completely normal when all grain boundaries become rough. The transition from AGG to normal growth with temperature increase is hence expected to be gradual as indeed observed in this work with the temperature increase from 1 100°C to 1 300°C.

**Miao *et al.* 🡪Olmsted *et al.* 🡪Yoon and Cho 🡪 Lee *et al*.:** *Note that the title of this article is “The dependence of AGG on initial grain size in 316 L stainless steel,” so I do not expect this article to discuss temperature in any specific detail.*

**Miao *et al.* 🡪Olmsted *et al.* 🡪Yoon and Cho 🡪 Koo and Yoon:** In Ni,[8]Ag,[11]and single-phase alloys[12,13]without any notable textures, AGG was observed to occur at relatively low temperatures when most of the grain boundaries were found to be faceted. At high temperatures close to melting points in certain atmospheres, the grain growth was found to be normal, with all of the grain boundaries defaceted and, hence, atomically rough.[8,11–14]Such a correlation between the grain-boundary structure and the grain-growth behavior was also found in such oxides as BaTiO3[15]and Al2O3.[16]