Grain Boundary Roughening Transition, and Its Effect on Sintering and Grain Growth

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Theoretical and experimental evidences for grain boundary roughening transition are reviewed. The roughening of crystal surface has been extensively studied. The solid-on-solid model predicts an infinite order roughening transition for crystal surface, where the step free energy and hence the area of the flat singular surface are predicted to decrease continuously to 0 at the roughening transition temperature T_R. The observed temperature dependence of surface structures, step free energy, and crystal shapes agree with these predictions. While T_R of the low index surfaces in some crystals may be higher than the bulk melting points T_m, T_R of grain boundaries are expected to be much lower except the symmetric twin boundaries and low angle grain boundaries. On the basis of calculated step energy and structural multiplicity, Rottman predicted grain boundary roughening transition at temperatures below T_m. When heat-treated at temperatures in the 0.5-0.7 T_m range, many grain boundaries in polycrystalline Ni, Cu, Ag, Ni-base superalloys, 316L stainless steel, an Fe-Si alloy, and Al_2O_3 are faceted with hill-and-valley or kinked shapes. Most of these flat grain boundary segments are expected to be singular and observed to be parallel to low index planes of the grains on either side. When heat-treated above 0.7 T_m, these grain boundaries become defaceted with curved shapes indicating their rough atomic structure. Similar defaceting grain boundary transitions have been observed also in Al and Au by Hsieh and Balluffi. Westmacott and Dahmen observed reversible rounding of flat grain boundary segments of island grains in Al, indicating singular-rough transition. The defaceting and roughening

transitions (and the reverse transitions) can also be induced by small amounts of additives as observed in Al_2O_3, $BaTiO_3$, Cu, Ni, and Fe. Numerous molecular dynamics simulations show continuous disordering of various grain boundaries to liquid-like structures at temperatures above about 0.5 T_m. This resembles the roughening transition behavior. The observed temperature dependence of other grain boundary properties such as diffusion, migration, grain growth, sliding, and precipitation also indicate grain boundary roughening transition at temperatures above about 0.5 T_m. It thus appears that all grain boundary segments exist in either singular or rough state corresponding to either flat or curved segments of grain boundary Wulff shapes at local equilibrium. The addition of small amounts of Ni to W appears to induce the roughening of both surfaces and grain boundaries, and hence the activated sintering effect. When the grain boundaries are singular, abnormal grain growth occurs because of the step growth mechanism. When the grain boundaries are rough, normal grain growth occurs because of the continuous migration mechanism.