THE RESTRUCTURING OF GRAIN BOUNDARIES AT THE SURFACES OF METALS

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Using a combination of atomically resolved scanning tunneling microscopy and computation we describe the restructuring of grain boundaries at metal surfaces. For all fcc metals we find that there is a strong preference for boundary cores to lie along close packed planes, regardless of the in plane misorientation angle of the boundary. However, since most fcc metals favour [111] growth, boundaries become locked in during the growth process leading to a preponderance of [111] tilt axes in the bulk. We show that there is a strong driving force to shift the tilt axes of these boundaries from [111] to [112] so that the cores can lie along close packed planes. This restructuring phenomenon is facilitated by the increased capacity for relaxation at free surfaces and has been observed to occur at the surfaces of both nanoscale and macroscopically thick metals. The depth of the restructuring depends on the misorientation angle and the shear modulus of the metal and can reach depths of over 10nm. For this reason, this phenomenon is expected to be very important in nanoscale materials where restructuring can persist throughout the materials depth (*Science* 357, 397-400 (2017)) and is expected to affect the mechanical properties of all metal materials on these length scales.