730 Finite temperature first principles calculations on Al <100> symmetric tilt and twist grain boundaries

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Finite temperature first principles calculations on Al <100> symmtetric tilt grain boundary energy were performed [1], and shows consistent results with the experimentally measured energy [2]. The effect of the finite temperature was obtained by the harmonic approximation of the Einstein model. The harmonic contributions are mainly controlled by the spring constant change due to the thermal expansion and the free volume around the edge dislocation. We also applied the same method on Al <100> symmetric twist boudnary, which shows the smaller temperature dependency than that of the tilt boundary.

[1] S. R. Nishitani, "Finite-temperature first-principles calculations of Al 〈100〉 symmetric tilt grain-boundary energy", Phil. Mag., 101 (2021), 622-642, https://doi.org/10.1080/14786435.2020.1855371.

[2] A. Otsuki, "Energies of [001] small angle grain boundaries in aluminum", J. Mater. Sci. 40 (2005), 3219-3223.

731 The top three superhard polycrystalline materials, their mechanical and optical properties

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Diamond, cubic boron nitride (cBN), and cubic silicon nitride (c-Si3N4) are known as the top three superhard materials. Diamond is the hardest material and the natural/man-made single crystals have been utilized as cutting tools and optical windows. Irifune et al. (2002) fabricated nanopolycrystalline diamond and the cutting tools with this material has been commercially available since 2012.

cBN is the second hardest and various types of polycrystalline cBN compacts with sintering additives have been fabricated and the cutting tools with these materials have been widely used for many industrial fields. Taniguchi et al. (1996) fabricated translucent polycrystalline cBN without additives using hBN as the starting material and reported the mechanical properties. However, the optical properties of this material have been barely studied.

Zerr et al. (1999) reported synthesis of c-Si3N4 with spinel structure under high pressure and temperature. Nishiayma et al. (2017) demonstrated that nanopolycrystalline c-Si3N4 shows optical transparency from ultraviolet to infrared wavelengths and that this material is the third hardest material.

In the presentation, I will first summarize the previous studies and industrial applications of the top three superhard polycrystalline materials. After that, I will introduce some newly obtained data of their mechanical and optical properties. I also discuss the potential future applications of these superhard polycrystalline materials.