Supporting Information

Pressure-Induced Structural Phase Transformation and Yield Strength of AlN

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Line-width analysis

The synchrotron radiation X-ray diffraction line profiles from the polycrystalline sample under nonhydrostatic uniaxial compression in a DAC exhibit broadening with increasing pressure. This broadening is attributed to two main factors: the reduction in grain size results in diffraction line broadening that varies with 1/cosθ, where θ is the diffraction angle; the broadening produced by the presence of micro-strains varies with tanθ. The theory of diffraction line broadening proposed earlier was derived from deformed metal and extended for the analysis of high pressure data at present[1-3]. The following formula describes the relation between the grain size and strain dependencies of diffraction line width：

$$(2\omega_{hkl}\cos\theta_{hkl})^2 = (\lambda/d)^2 + {\eta_{hkl}}^2\sin^2\theta_{hkl}, \tag{1}$$

where $2\omega_{hkl}$ is the full-width at half-maximum (FWHM) of the diffraction profile. The symbles λ, d, η_{hkl} denote the X-ray wavelength, sample grain size, and the microscopic deviatoric strain, respectively. The micro-strains can be obtained from the following relation:

$$\eta_{hkl}^2 = \left[(2\omega_{hkl}\cos\theta_{hkl})^2 - (\lambda/d)^2\right]/\sin^2\theta_{hkl}, \tag{2}$$

The expression for the (*hkl*)-dependence of η_{hkl} was made under the assumption that all of the stresses between 0 and p_{max} in the crystallite are possibly equal. The relation proposes that η_{hkl} depends on *E(hkl)*, so the Young's modulus values are in conformity to the following relation in the direction [h k l]:

$$\eta_{hkl} = 4p_{max}/E(h\,k\,l), \quad (3)$$

The p_{max} could be calculated by η_{hkl} using Eq. (3) when the elastic moduli of single crystals are known. The aggregate *E* can be obtained from the bulk modulus *K* and the shear modulus *G* by the following relation:

$$E = 9KG/(3K + G). \quad (4)$$

Many other materials[3, 4] suggest that t obtained from the line-shift analysis and p_{max} obtained from the line-width analysis satisfy the relation $2p_{max} \cong t$. Both t and $2p_{max}$ are taken as measures of compressive strength. The yield strength *Y* can thus be obtained from the following relation：

$$Y = t = \varepsilon E. \quad (5)$$

where ε is the average value of η_{hkl}.

References

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