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# Supplementary Material

# Fracture Toughness and Critical Thickness of β-$(In_xGa_{1-x})_2O_3$ / $Ga_2O_3$ by First Principles

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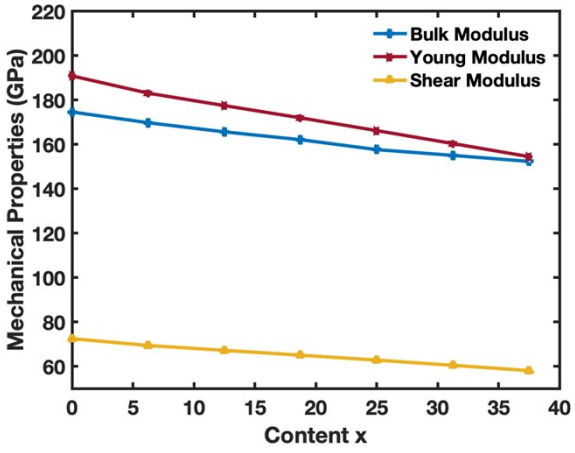
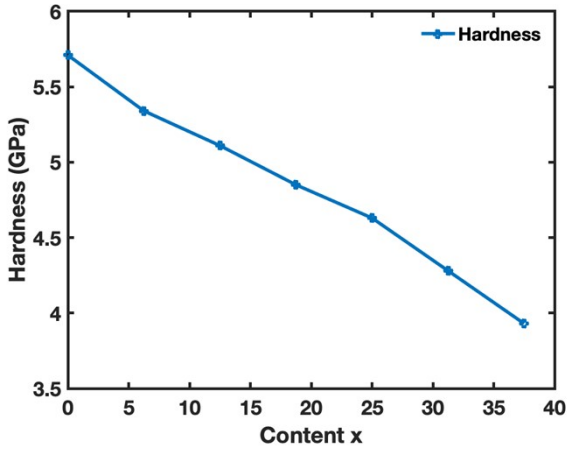



Supplementary Fig. 1. Mechanical properties of $Ga_2O_3$ and $(In_xGa_{1-x})_2O_3$ with In concentration up to 37.5%. Blue line represents bulk modulus, red line represents Young's modulus and yellow line represents shear modulus.




Supplementary Fig. 2. Hardness of $Ga_2O_3$ and $(In_xGa_{1-x})_2O_3$ with In concentration up to 37.5%.

Table I: Poisson's Ratio of $Ga_2O_3$ and $(In_xGa_{1-x})_2O_3$ with In concentration up to 37.5%.

| **In Content** | **0.00%** | **6.25%** | **12.50%** | **18.75%** | **25.00%** | **31.25%** | **37.50%** |
|---|---|---|---|---|---|---|---|
| **Poisson's Ratio** | **0.32** | **0.32** | **0.32** | **0.32** | **0.32** | **0.33** | **0.33** |

The in-plane and out-of-plane strain for [010] orientation:

$$\epsilon_{xx} = \frac{a_s}{a_f} - 1$$

$$\epsilon_{zz} = \frac{c_s sin\beta_s}{c_f sin\beta_f} - 1$$

$$\epsilon_{xz} = \frac{(a_f - a_s)cos\beta_f}{2a_f sin\beta_f} + \frac{c_s cos\beta_s - c_f cos\beta_f}{2c_f sin\beta_f} = \frac{1}{2}\left(\frac{c_s sin\beta_s}{c_f sin\beta_f} - \frac{a_s}{a_f} cot\beta_f\right)$$

For the surface conditions $\sigma_{yy} = \sigma_2 = 0$ and $\sigma_4 = \sigma_6 = 0$, $\epsilon_{xy} = \epsilon_{yz} = 0$ and

$$\epsilon_{yy} = -\frac{C_{12}\epsilon_{xx} + C_{23}\epsilon_{zz} + 2C_{25}\epsilon_{xz}}{C_{22}}$$

The in-plane and out-of-plane strain for [100] orientation:

$$\epsilon_{xx}^{'} = \frac{c_s}{c_f} - 1$$

$$\epsilon_{yy}^{'} = \epsilon_{yy} = \frac{b_s}{b_f} - 1$$

Angle $\theta$ is the angle of (100) plane against z-direction.

$$\epsilon_{xx} = \epsilon_{xx}^{'} cos^2\theta + \epsilon_{zz}^{'} sin^2\theta - 2\epsilon_{xz}^{'} cos\theta sin\theta$$

$$\epsilon_{zz} = \epsilon_{xx}^{'} sin^2\theta + \epsilon_{zz}^{'} cos^2\theta - \epsilon_{xz}^{'} sin2\theta$$

$$\epsilon_{xz} = (\epsilon_{xx}^{'} - \epsilon_{zz}^{'}) cos\theta sin\theta + \epsilon_{xz}^{'} cos2\theta$$