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Elastic moduli, anisotropy and refractive index of γ -Ge₃N₄ via laser ultrasonics, Brillouin light scattering, and first-principles calculations

Dr. Chen-Hui Li¹, Prof. Philippe Djemia¹, Dr. Nikolay Chigarev², Ms. Siham Sodki¹,
Prof. Yves Roussigné¹, Prof. Samuel Raetz², Prof. Vitaliy E. Gusev², Dr. Andreas Zerr¹

¹Laboratoire des Sciences des Procédés et des Matériaux - CNRS, Villetaneuse, France, ²Laboratoire d'Acoustique de l'Université du Mans, Le Mans, France

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Germanium nitride having cubic spinel structure, γ -Ge₃N₄, is a wide band-gap semiconductor, $E_g=3.65(5)$ eV, with a large exciton binding energy [1,2] which exhibits high hardness, elastic moduli and elevated thermal stability to $\sim 700^\circ\text{C}$. Experimental data on its bulk and shear moduli (B_0 and G_0 , respectively) are strongly limited [3–6], inconsistent and, thus, require verification. Moreover, earlier first-principles density functional calculations provided significantly scattering B_0 values but consistently predicted G_0 much higher than the experimental one [7–9]. Here, we investigated the elastic behaviour of γ -Ge₃N₄ experimentally, using the techniques of laser ultrasonics (LU) and Brillouin light scattering (BLS), and theoretically, using the first-principles calculations. We measured velocities of the Rayleigh surface acoustic waves (RSAWs) and of the longitudinal acoustic waves (LAWs) in our low-porosity polycrystalline sample using the LU-technique and derived its isotropic elastic moduli B_p and G_p (here and below, the subscripts p and 0 indicate values for the porous and densified sample, respectively). Applying the Hashin-Shtrikman approach, we obtained $B_0=322(44)$ GPa and $G_0=188(7)$ GPa for the dense γ -Ge₃N₄. The significant error in B_0 is explained by the low amplitude of the LAW-signals in our LU-measurements. Nevertheless, it agrees, within experimental uncertainties, with the $B_0=295(5)$ GPa [3] obtained from the EOS measured upon quasi-hydrostatic compression. Both the previous and the present first-principles calculations underestimated B_0 while the GGA-PBEsol functional with a hard PAW potential showed the least deviation from the experiment.

Our experimental G_0 exceeds by ~ 1.5 times the previous experimental value, $G_0=124$ -129 GPa derived from the nanoindentation testing [4, 5]. The calculated G_0 values, typically around 170 GPa, were underestimated but much less significant than the B_0 , between 211-269 GPa. However, $G_0=186(10)$ GPa calculated using the GGA-PBEsol functional with a hard PAW potential agreed with our measurements. Comparison of the RSAW-velocity values, VR_0 , measured using the LU- and BLS techniques confirmed the theoretically-predicted elastic anisotropy of γ -Ge₃N₄. The anisotropy led to the asymmetric RSAW peaks in our BLS measurements resulting in the VR_0 underestimation by $\sim 10\%$. Combining our LU- and BLS results for the LAWs, we determined the refractive index of the dense γ -Ge₃N₄ to be $n_0=2.4(1)$. This value ranks γ -Ge₃N₄ in the class of very-high-refractive-index materials transparent for visible light, such as diamond, GaN or TiO₂ having anatase structure.

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