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► **To cite this version:**

Andreas Zerr, Feng Xu, Philippe Djemia, Y. Roussigné. Influence of elastic anisotropy on measured sound velocities of cubic solids. The Joint 28th AIRAPT and 60th EHPRG International Conference 2023, Jul 2023, Edinburgh, Scotland, United Kingdom. pp.157. hal-04241739

HAL Id: hal-04241739

<https://hal.science/hal-04241739v1>

Submitted on 13 Oct 2023

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Influence of elastic anisotropy on measured sound velocities of cubic solids

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Instrumentation and Techniques 4, July 26, 2023, 16:30–18:30

Pressure dependences of the longitudinal sound velocities, $V_L(P)$, single-crystal elastic moduli, $C_{ij}(P)$, and elastic anisotropy, described through the Zener anisotropy ratio $A=2C_{44}/(C_{11}-C_{12})=C_{44}/C'$, of three simple cubic solids, namely, solid argon, cubic H₂O ice and NaCl (B1-phase) were recently measured using the technique of the picosecond laser ultrasonics (ps-LU) [1-4]. These experiments revealed growing with pressure elastic anisotropy: $A\approx 6$ for argon at $P=49$ GPa, $A\approx 6.5$ for H₂O-ice VII at 62 GPa, $A\approx 0.27$ for NaCl-B1 at $P=28$ GPa. The latter manifested itself in diverging of the VL-extremes in single crystals corresponding, in cubic crystals, to the crystallographic directions $\langle 111 \rangle$ and $\langle 100 \rangle$, while $V_{L111} > V_{L100}$ if $A > 1$ and vice-versa if $A < 1$. Moreover, the $V_{Lav}(P)$ dependences measured for polycrystalline samples of these solids using Brillouin light scattering (BLS) e.g.[5-7] were found to approach $V_{L110}(P)$, independent of the $A(P)$ value, and to deviate from the $V_{LH}(P)$ dependences calculated applying the experimental $C_{ij}(P)$ and the Hill approximation. Here, we show that the latter inconsistency is caused by the elastic anisotropy and that the BLS provides overestimated longitudinal and transversal sound velocities of polycrystalline cubic solids, $V_{Lav}(P)$ and $V_{Tav}(P)$, respectively, if $A > 1$ and underestimated $V_{Lav}(P)$ and $V_{Tav}(P)$ if $A < 1$. However, the chance to recognise BLS-peaks of transversal waves in the polycrystalline solids decreases with increasing elastic anisotropy due to the peak broadening and splitting [3]. Distortion of the peaks of the longitudinal waves is less pronounced but still significant.

We evaluated the influence of such distortion on the aggregate shear modulus, $G_{av}(P)$, derived from the $V_{Lav}(P)$ and the bulk modulus, $B(P)$, obtained from an EOS. For solid Ar at $P=49$ GPa, we found that G_{av} deviates from G_H by $\sim 50\%$. Furthermore, our LU- and BLS-measurements on polycrystalline γ -Ge₃N₄ having spinel structure [8] confirmed that the elastic anisotropy also influenced position and shape of the Rayleigh peak in the BLS measurements. In general, V_{Rav} is underestimated if $A > 1$ and overestimated if $A < 1$. Our evaluation of the influence of anisotropy on the BLS-peaks of γ -Ge₃N₄, with calculated $A=2.1$ [9], resulted in G underestimated by $\sim 9\%$ and B overestimated by $\sim 29\%$.

However, similar limitations are relevant for any technique measuring sound velocities with probes having sizes comparable with those of the sample grains. The most reliable approach remains measurement of $C_{ij}(P)$ and extraction of the values of interest using the Hill (or similar) approximation. The ps-LU meets well this requirement at high pressures, also in excess of 100 GPa, because its high 3D-resolution makes use of single crystals unnecessary.

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28th AIRAPT and 60th EHPRG

23–28 July 2023

Edinburgh International Conference Centre,
Edinburgh, UK

