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Lattice dynamics of NaAlH$_4$ from high-temperature single-crystal Raman scattering: Evidence of highly stable AlH$_4^-$ anions

ERIC MAJZOUB, KEVIN MCCARTY, Sandia National Laboratories, VIDVUDS OZOLINS, UCLA — Polarized Raman scattering on single crystals of NaAlH$_4$ has been used to determine the symmetry properties and frequencies of the Raman-active vibrational modes over the temperature range from 300 to 425 K, i.e., up to the melting point $T_{\text{melt}}$. Significant softening (by up to 6%) is observed in the modes involving rigid translations of Na$^+$ cations and translations and librations of AlH$_4^-$. Surprisingly, the data indicate mode softening of less than 1.5% for the Al-H stretching and Al-H bending modes of the AlH$_4^-$ anion. These results show that the AlH$_4^-$ anion remains a stable structural entity even near the melting point. The enhanced kinetics of absorption and desorption in Ti-doped NaAlH$_4$ powders is attributed to the effectiveness of Ti in promoting the break-up of the AlH$_4^-$ anions.

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