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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_{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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