

Abstract Submitted
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Strong negative thermal expansion in metal carbides using the quasi-harmonic approximation¹ PINKU NATH, JOSE J. PLATA, DEMET USANMAZ, Duke University, MARCO FORNARI, Central Michigan University, MARCO BUONGIORNO NARDELLI, University of North Texas, STEFANO CURTAROLO, Duke University — Negative thermal expansion (NTE) is a very rare but important property found in materials in which they shrink upon heating. Negative and positive thermal expansion substances can be combined to synthesize zero thermal expansion composites. There are very few compounds with very strong NTE for a wide range of temperatures. For instance, network structured compounds such as $(\text{Zr,Hf})\text{W}_2\text{O}_8$, show an isotropic NTE for a wide range of temperature larger than 1000 K. However, strong NTE materials without a network structure are very rare. Here, we have studied the thermal expansion of transition metal carbides using the quasi-harmonic approximation. Their phonon dispersion curves show low energy (less than 8 meV) transverse acoustic modes observed as intense and sharp peaks in their phonon density of states. These compounds present large negative Grüneisen parameters for their transverse acoustic bands, which is reflected in the intense NTE behavior from close to 0 K to more than 1000 K.

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