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Ab initio phase stability at high temperatures and pressures in the V-Cr system ALEXANDER LANDA, PER SODERLIND, LIN YANG, Lawrence Livermore National Laboratory — Vanadium metal has seen a surge in research, experimental and theoretical, driven mainly by its importance in applications but also because of its surprising destabilization of the body-centered cubic (bcc) ground-state phase close to 60 GPa. The phase stability of vanadium metal and vanadium-chromium alloys at high temperatures and pressures is explored by means of first-principles electronic-structure calculations. Utilizing the self-consistent *ab initio* lattice dynamics approach in conjunction with density-functional theory, we show that pressure-induced mechanical instability of body-centered cubic vanadium metal, which results in formation of a rhombohedral phase at around 60 GPa at room temperatures, will prevail significant heating and compression. Furthermore, alloying with chromium decreases the temperature at which stabilization of the body-centered cubic phase occurs at elevated pressure. Computing support for this work came from the LLNL Computing Grand Challenge program. This work performed under the auspices of the U.S. DOE by LLNL under Contract DE-AC52-07NA27344 and funded by the Laboratory Directed Research and Development Program at LLNL under project tracking code 11-ER-033.

Alexander Landa
Lawrence Livermore National Laboratory

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