Fermi surface nesting and pre-martensitic softening in V-Nb system under high pressure[1] ALEXANDER LANDA, JOHN KLEPEIS, PER SODERLIND, BABAK SADIGH, Lawrence Livermore Nationa Laboratory, Livermore, CA 94550, IVAN NAUMOV, University of Arkansas, Fayetteville, AR 72701, OLEG VELIKOKHATNYI, Carnegie Mellon University, Pittsburgh, PA 15213, LEVENTE VITOS, ANDREI RUBAN, Royal Institute of Technology, SE-10044, Stockholm —

First-principles total energy calculation based on the exact muffin-tin orbital and full potential linear muffin-tin orbital methods were used to calculate the equation of state and shear elastic constants of bcc V, Nb, and the $V_{95}Nb_{05}$ disordered alloy as a function of pressure up to 6 Mbar. We found a mechanical instability in C_{44} and a corresponding softening in $C^{'}$ at pressures $\sim$ 2 Mbar for V. Both shear elastic constants show softening at pressures $\sim$ 0.5 Mbar for Nb. Substitution of 5 at. % of V with Nb removes the instability of V with respect to trigonal distortions in the vicinity of 2 Mbar pressure, but still leaves the softening of C_{44} in this pressure region. We argue that the pressure induced softening in the shear elastic constants of V and Nb can be attributed simultaneously to three different electronic structure peculiarities, namely to the Fermi Surface nesting, electronic topological transition, and the band Jahn-Teller effect.

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