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Shock Compression of Niobium Oxides from First-Principles

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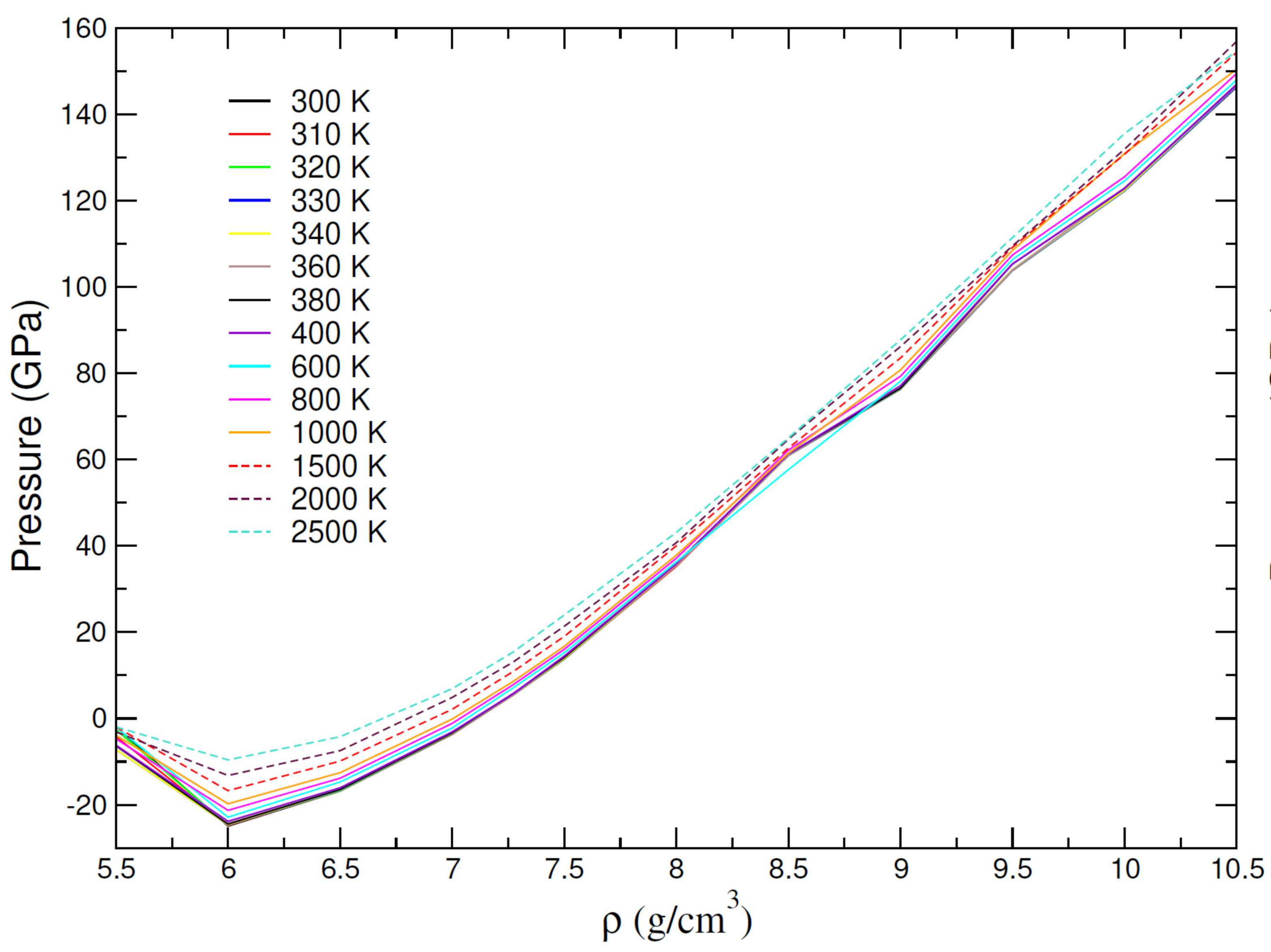
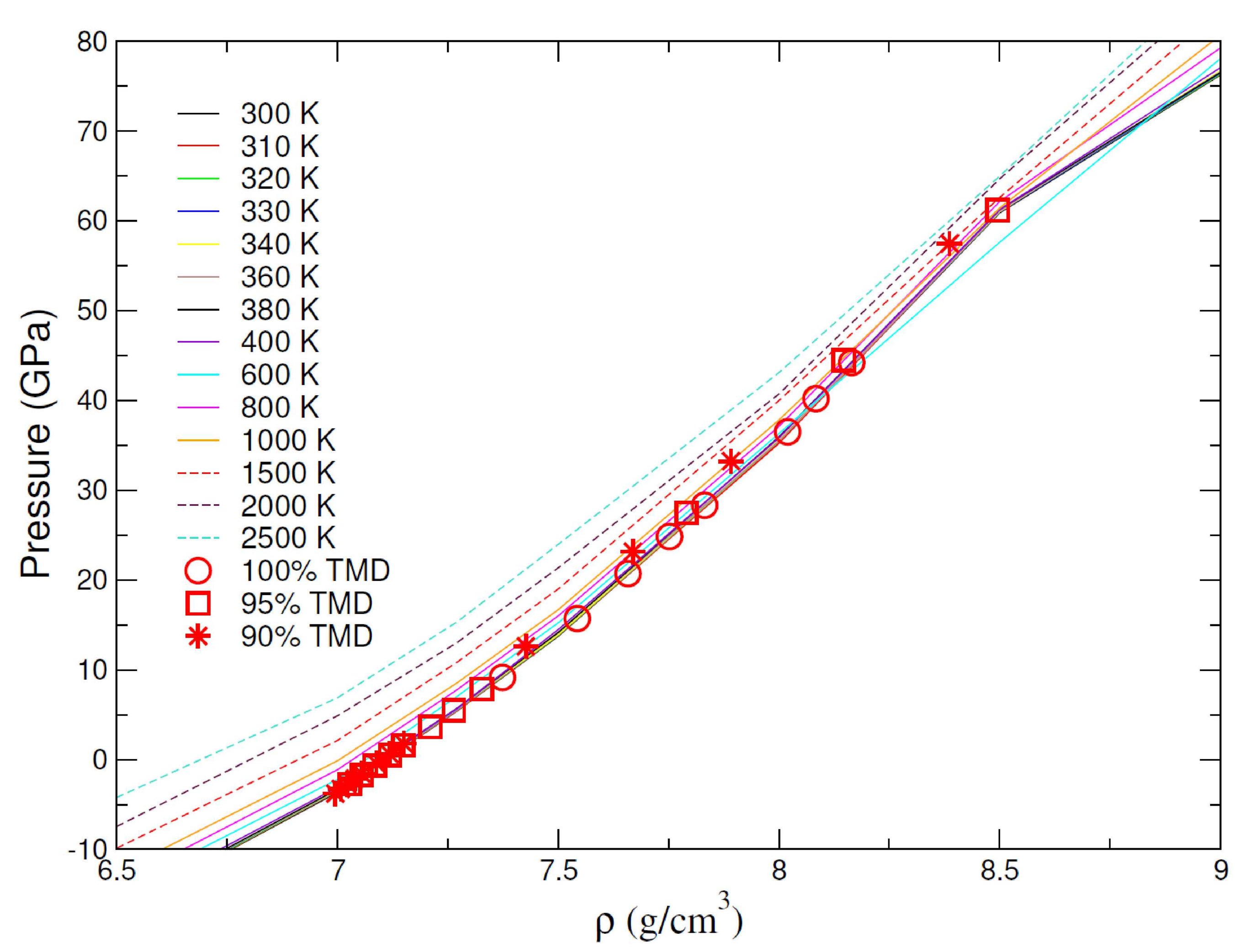
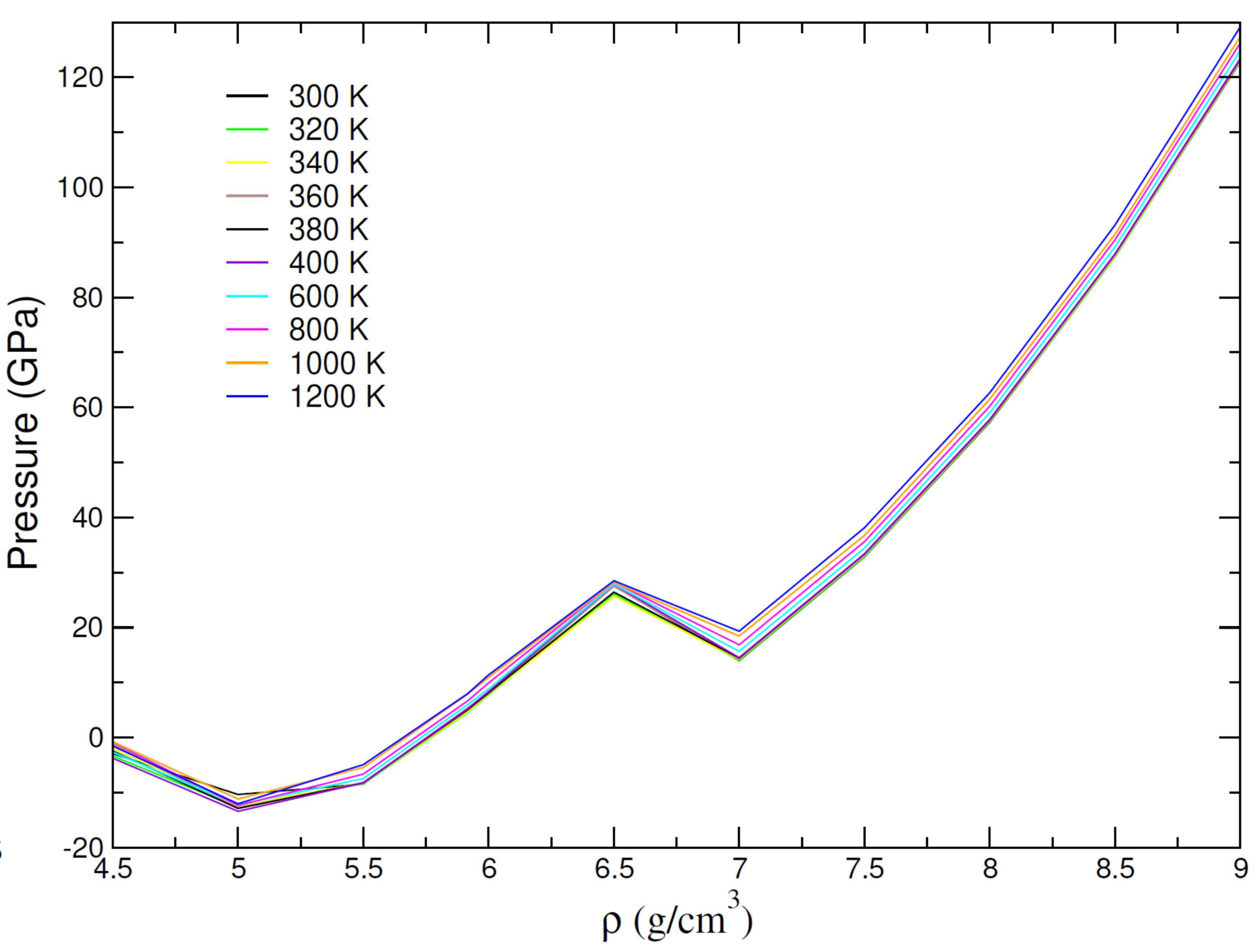
- To assess the impact of oxidation on the properties of niobium subjected to shock loading, the equations of state (EOS) and shock properties of bulk NbO and NbO_2 were predicted from ab initio molecular dynamics (AIMD) simulations.
- NbO forms during the initial rapid oxidation of Nb films and crystallizes in the cubic Pm3-m structure. NbO_2 adopts a tetragonal superstructure with a subcell of the rutile type, with space group $I4_1/a$. 48-atom and 96-atom supercells were used to simulate NbO ($\rho_0 = 7.27$ g/cm^3) and NbO_2 ($\rho_0 = 5.92$ g/cm^3).

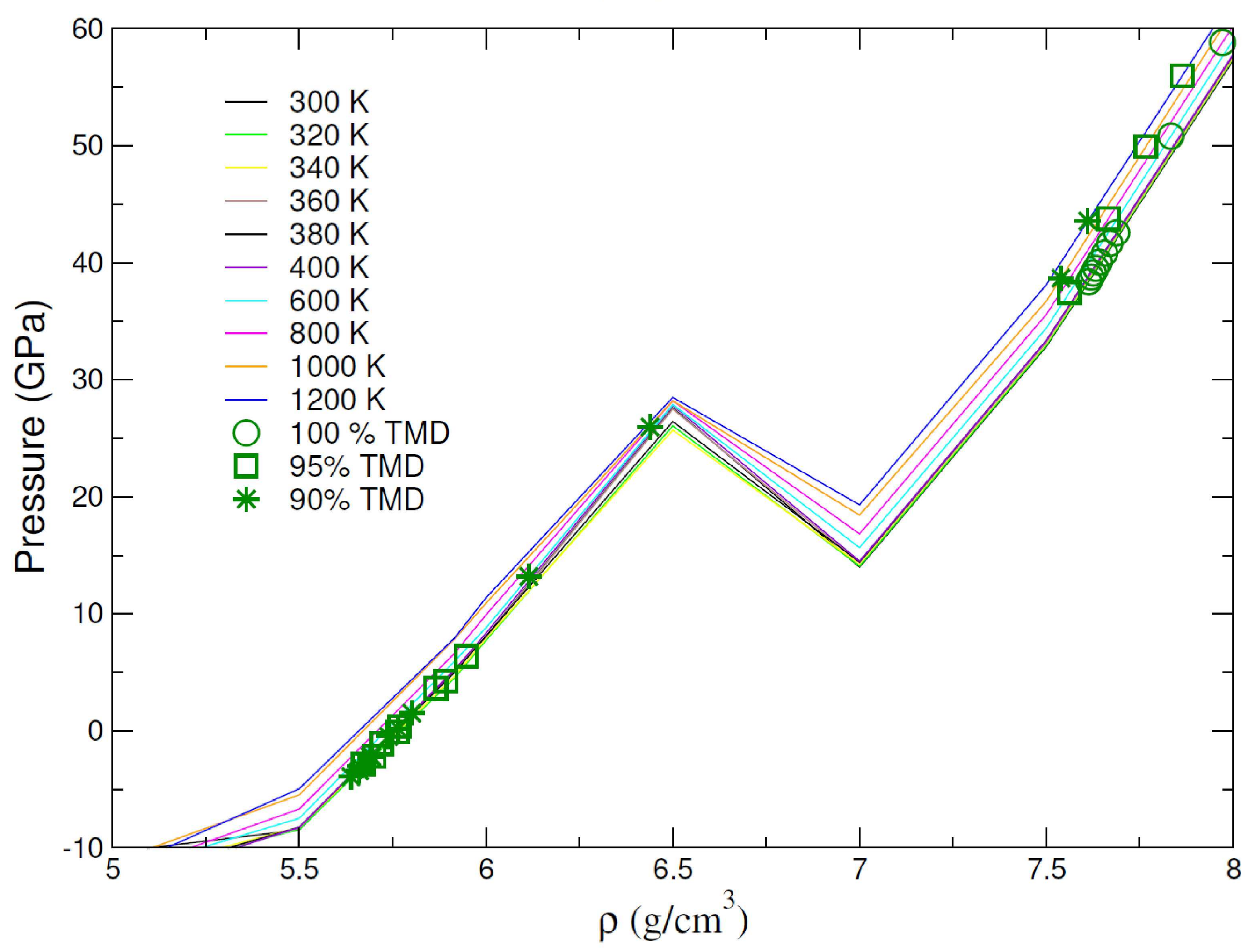
NbO EOS





NbO_2 EOS



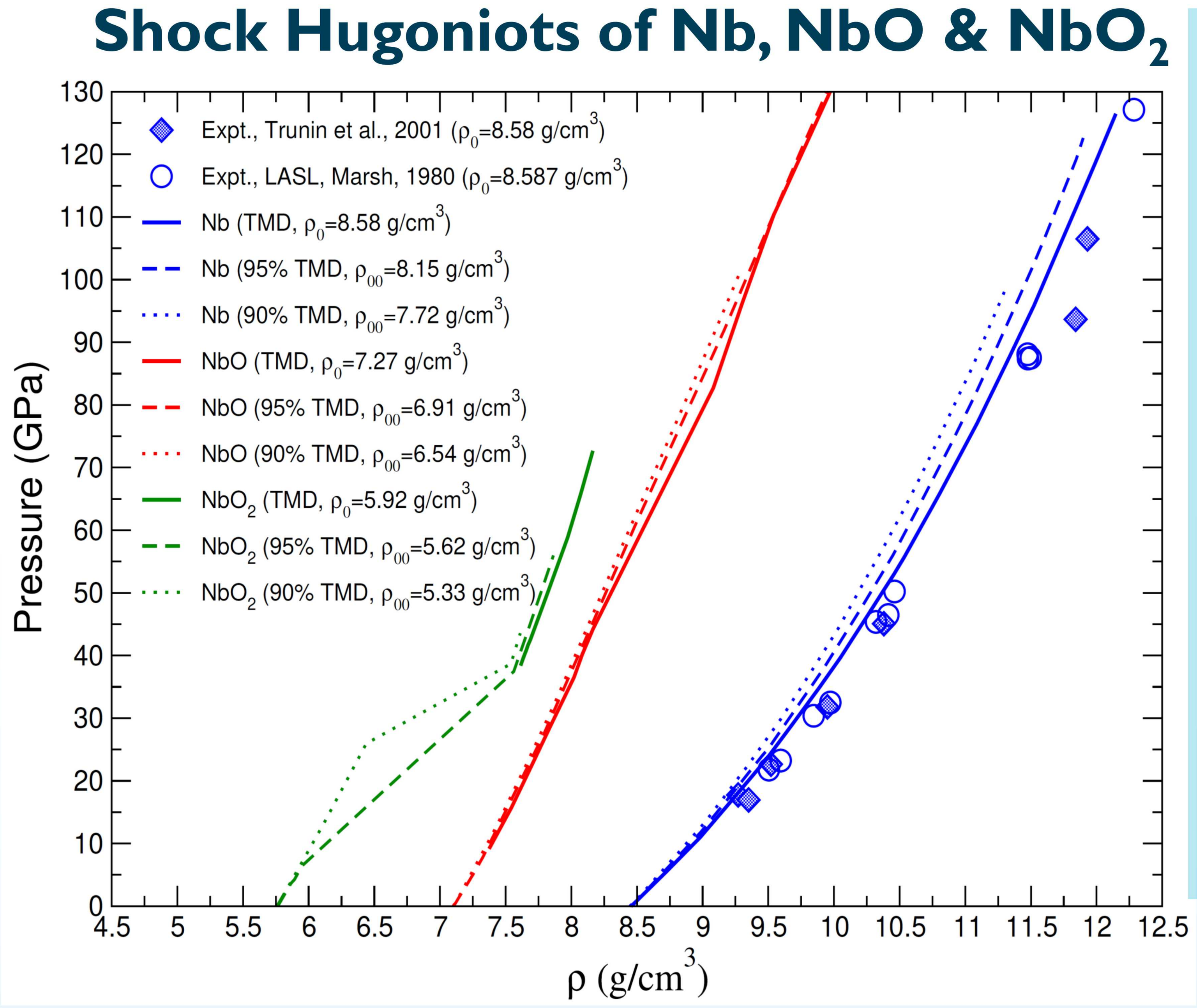


- AIMD simulations conducted using spin-polarized DFT with the Vienna ab initio simulation package (VASP).
- PBE XC functional, with projector augmented wave (PAW).
- Canonical (NVT ensemble) simulations to calculate isotherms in the ranges 300-2500 K for NbO and 300-1200 K for NbO_2. ρ = 5.5-10.5 g/cm^3 and 4.5-9.0 g/cm^3, in increments of 0.5 g/cm^3 in AIMD simulations of pure NbO and NbO_2.
- Baldereschi's mean-value special k-point for properties averaging in the Brillouin zone.
- 0.7 fs time step for ion-motion.
- Hugoniot curve consists of (P; V; T) points satisfying the Hugoniot relation:

$$E - E_0 + (1/2)(P + P_0)(V - V_0) = 0$$

E: specific internal energy;
P: pressure; $V = 1/\rho$
E_0, P_0, V_0: reference energy, pressure and volume at 300 K.
For initially porous oxides (ρ_{00}), V_0 above is replaced with $V_{00} = 1/\rho_{00}$.

Shock Hugoniots of Nb, NbO & NbO_2



- NbO and NbO_2 isotherms show possible phase transitions above 60 GPa and 30 GPa, respectively. Further confirmation using simulations and experiments is needed to identify and characterize these transitions.
- At lower pressure, the effect of oxidation remains relatively limited according to the present AIMD simulations. α-to-β and β to baddeleyite-type transitions in NbO_2 were not seen in AIMD simulations [1] and NbO did not appear to disproportionate [2].
- An extensive study of Nb_2O_5 polymorphs subjected to shock loading might be necessary to completely rule out any detrimental effect from higher oxidation.
- The results of this study also indicate that, for the application of weak and intermediate shocks, the tabular EOS models generated from AIMD simulations are expected to provide reliable predictions.

References

[1] Haines et al., Phys. Rev. B, 59, 13650 (1999)
[2] D'yachkova et al., Zhur. Neorganich. Khim., 31, 1879 (1986)

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