Supplementary Material

1. DFT calculated physical properties of $Mo_{10}Ni_3C_3B$

$Mo_{10}Ni_3C_3B$ phase has a hexagonal crystal structure with P63/mmc space group (Fig. S1), where atoms occupied the positions of 12k (0.20, 0.40, 0.07), 6h (0.55, 0.10, 0.25), 2a (0, 0, 0) — 3 positions of Mo, 6h (0.89, 0.78, 0.25)-Ni, 6g (0.25, 0, 0)-C and 2c (0.33, 0.67, 0.25)-B. The unit cell contains two formula units of the phase and includes 34 atoms: $Mo_{20}Ni_6C_6B_2$.

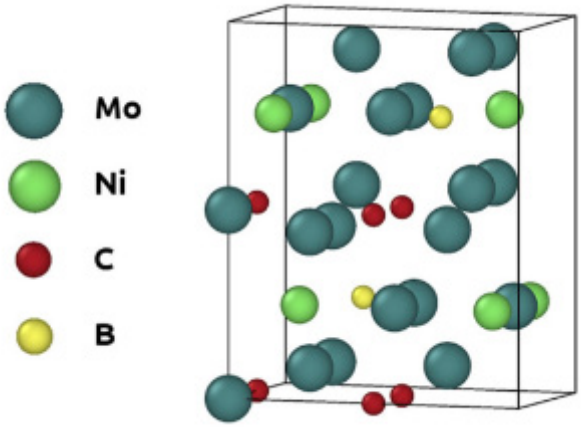

Fig. S1. Structure of 34-atom unit cell of $Mo_{10}Ni_3C_3B$ phase.

Fig. S2 displays the calculated phonon dispersion curves of our phase. The dynamical stability is further demonstrated by the phonon-density-of-state (PhDOS). The absence of negative frequencies in Fig. S2 also means the mechanical stability of the $Mo_{10}Ni_3C_3B$ phase.

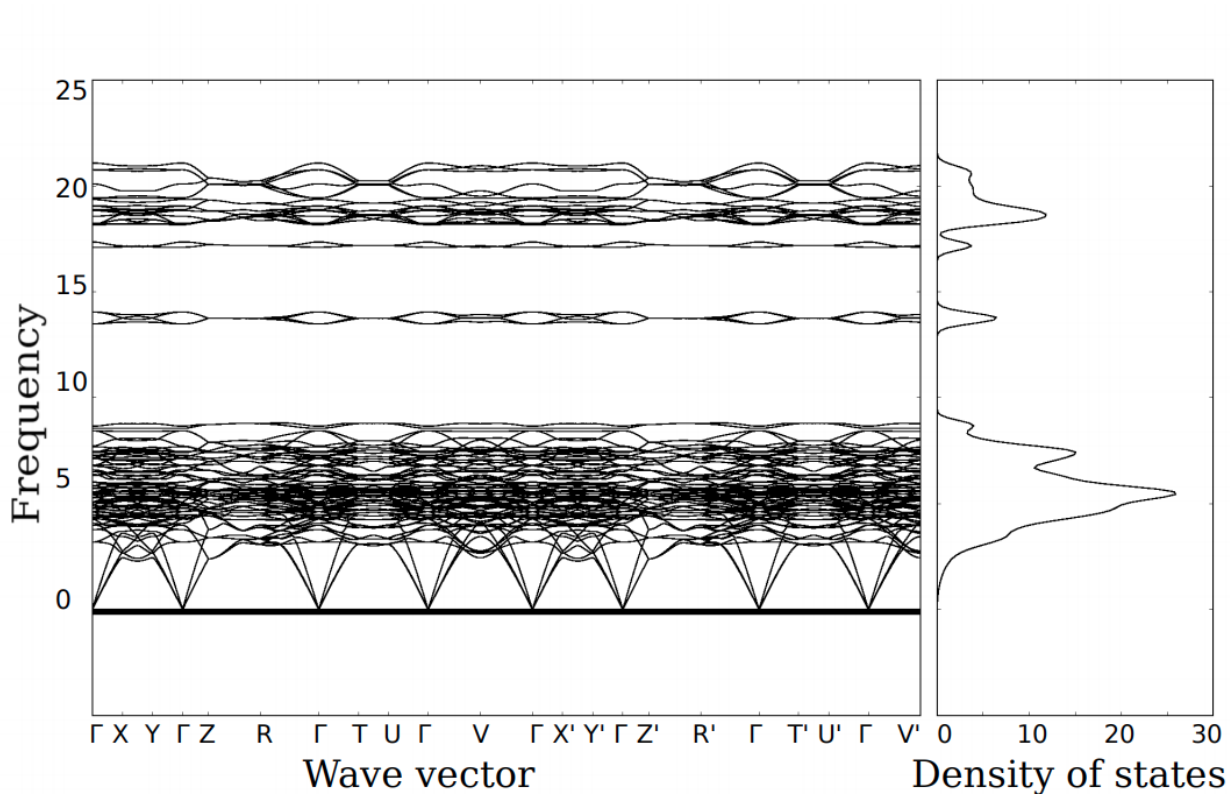

Fig. S2. Phonon dispersion curves and phonon density of state of $Mo_{10}Ni_3C_3B$ phase.

https://doi.org/10.22226/2410-3535-2020-4-387-391

Fig. S3 shows the total density of states (TDOS) and partial density of states (PDOS) near the Fermi level (E_F) defined as 0 eV. As shown, the TDOS values are positive at E_F for considered phase, indicating metallic character to some degree [24].

Fig. S4 shows the calculated phonon free energy, entropy, and heat capacity at constant volume (CV) per unit cell of the $Mo_{10}Ni_3C_3B$ phase as a function of temperature. Vibrational zero-point energy (ZPE) per unit cell is 44.76 kJ/mol, vibrational entropy in harmonic limit and heat capacity at constant volume are 1903.83J/K/mol and 443.82 J/K/mol, respectively.

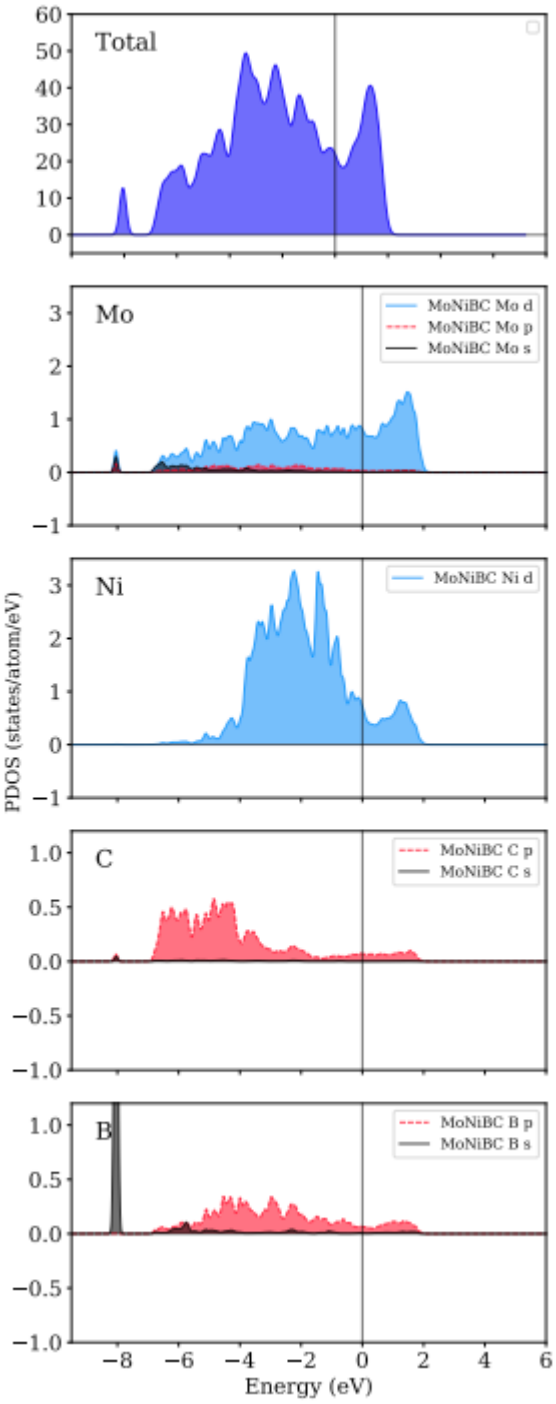

Fig. S3. Total DOS of $Mo_{10}Ni_3C_3B$ phase and partial DOS of elements near the Fermi level (0 eV).

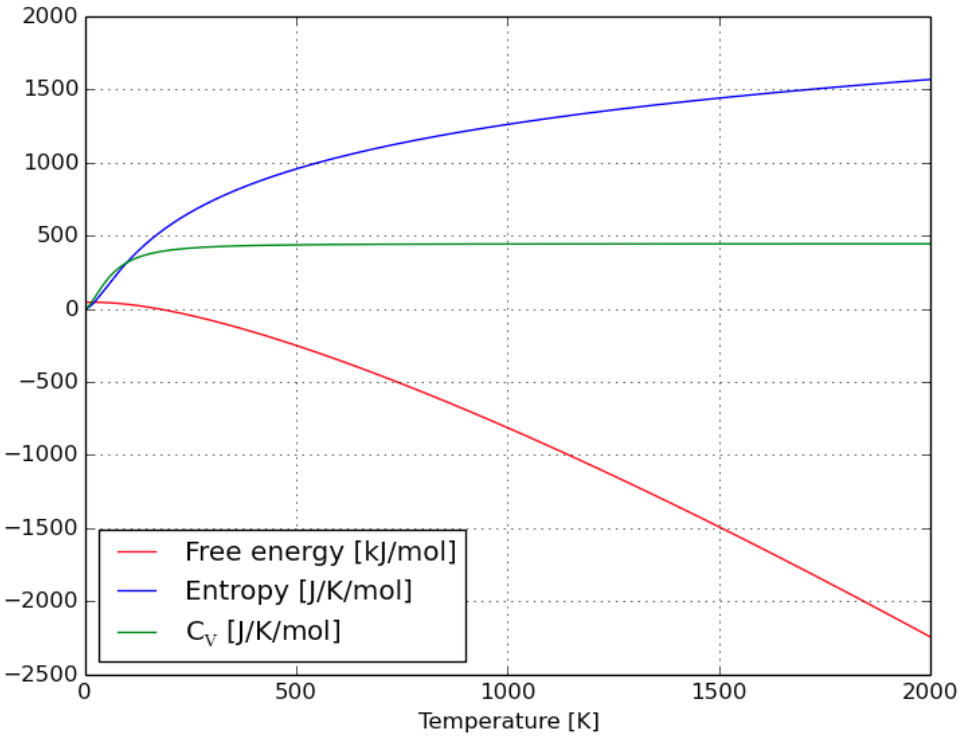

Fig. S4. Thermal properties of $Mo_{10}Ni_3C_3B$ phase.

2. Calculation details

The bulk modulus, shear modulus, Young's modulus, and Poisson's ratio were estimated according to Hooke's law and the Voigt-Reuss-Hill (VRH) model [25 – 26]. For hexagonal polycrystalline crystal:

$$B = [2(C_{11} + C_{12}) + 4C_{13} + C_{33}]/9,$$
$$G = (C_{11} + C_{12} + 2C_{33} - 4C_{13} + 12C_{44} + 12C_{66})/30,$$
$$E = 9BG/(3B + G),$$
$$\nu = (3B - 2G)/2(3B + G),$$

The Vickers hardness (HV) was calculated according to the empirical formula [19]:

$$HV = 2(K^2G)0.585 - 3,$$
$$K = G/B.$$

The values of universal anisotropy factor (A^U) and anisotropy factor of shear modulus (A^G), which are associated with plastic deformation, have been calculated in agreement with [17, 27] and shown below:

$$A^U = 5(G_V/G_R) + (B_V/B_R) - 6 \geq 0$$
$$A_G = (G_V - G_R)/(G_V + G_R),$$

where B_V (B_R) and G_V (G_R) are bulk and shear moduli in Voigt [28] (Reuss [29]) approximation, respectively.

References

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