

Electronic Supplementary Material

Water-based lubrication of niobium nitride

Kaifei MIAO¹, Jia WANG^{2,*}, Qiang ZHAO¹, Kaiwen WANG¹, Mao WEN¹, Kan ZHANG^{1,*}

¹ State Key Laboratory of Superhard Materials, Department of Materials Science, Key Laboratory of Automobile Materials, MOE, Jilin University, Changchun 130012, China

² Department of Materials Science and Engineering, Jilin Jianzhu University, Changchun 130118, China

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Nanoindentation was performed to explore the mechanical properties of NbN. As shown in Fig. S1, both curves have a tendency of increasing first and then decreasing to various degrees resulting from the effect of surface and substrate, respectively. The intrinsic values in the hardness (Fig. S1(a)) and elasticity modulus (Fig. S1(b)) can be averaged within the first 40–90 nm indentation (colored shaded rectangle region) to avoid those effects. The obtained values are about 23.74 ± 0.58 GPa and 288.33 ± 4.48 GPa, respectively.

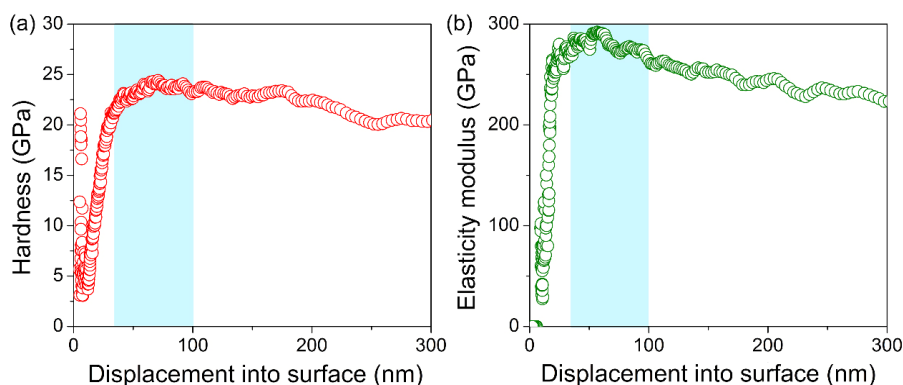


Fig. S1 (a) Hardness–displacement curve and (b) elasticity modulus–displacement curve for NbN.

Figure S2 shows the change curves of viscosity and shear stress corresponding to shear rate. When the shear rate is less than 0.25 s^{-1} , the viscosity of “colloidal solution” increases first and then decreases with the increase of shear rate. At this time, the “hydration layer” consisting of “colloidal solution” belongs to a non-Newtonian fluid flow mode. The reason for the shearing dilution in the initial stage may be due to the decomposition of the micropolymers in the liquid [S1]. In the “colloidal solution”, with the increase of shear rate, the binding force between colloidal particles is weakened and the colloidal deformations occur, which reduces the interconnection between colloidal particles and leads to the overall decrease of viscosity. This characteristic of “colloidal solution” helps to reduce the shear resistance caused by the viscous divergence of larger viscosity [S2]. When the shear rate is greater than 0.5 s^{-1} , the viscosity of “colloidal solution” no longer changes with the change of shear rate, and basically remains at $32.05 \text{ mPa}\cdot\text{s}$. Under this condition, the shear stress fluctuates in a very small range with the change of shear rate, showing an approximately linear upward trend. The friction linear velocity used in our work is 1 cm/s , the corresponding shear rate is 0.796 s^{-1} , and the “hydration layer”

* Corresponding authors: Kan ZHANG, E-mail: kanzhang@jlu.edu.cn; Jia WANG, E-mail: wangjia@jlu.edu.cn

consisting of “colloidal solution” presents the Newtonian fluid feature. Compared with pure water (about 0.89 mPa·s at 25 °C), “colloidal solution” have a higher viscosity, which improves the poor film-forming and lubricating abilities of interfacial water due to its low viscosity [S3]. In addition, the continuous fluidity of colloidal solution is also better.

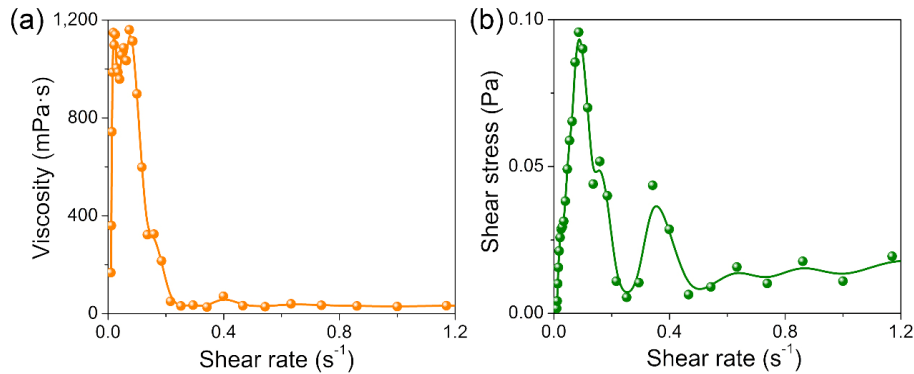


Fig. S2 (a) Viscosity and (b) shear stress of “colloidal solution” at room temperature as a function of shear rate.

To clarify the lubrication regime during the low friction period, the film thickness (h_c) between tribopairs and the lambda-ratio (λ) have been calculated. The corresponding curves of viscosity and shear rate were obtained by rotating rheological test of “colloidal solution”. As shown in Fig. S2, when the shear rate exceeds 0.25 s^{-1} , the liquid viscosity stabilizes at about 32.05 mPa·s. The frictional linear velocity of 1 cm/s corresponds to the shear rate of 0.796 s^{-1} , so the viscosity of “colloidal solution” is about 32.05 mPa·s during the tribo-test. Then, a detailed calculation of lambda-ratio (λ) for the tribo-contact has been performed, as follows:

During the low friction period, the film thickness (h_c) between the tribopairs was calculated using the Hamrock–Dowson Eq. (S1) [S4]:

$$h_c = (2.69G^{0.53}RU^{0.67}/W^{0.067}) \cdot (1 - 0.61e^{-0.73k}) \quad (\text{S1})$$

where $G = \alpha E'$, $U = \eta u/E'R$, $W = F/E'R^2$, and $k \approx 1$ is a coefficient and α refers to the pressure–viscosity coefficient of the lubricant, which is usually in the range of 4–8 GPa⁻¹ for water-based lubricants [S5]. The viscosity (η) is 32.05 mPa·s for “colloidal solution”. In this paper, the applied load (F) and average velocity (u) are 1 N and 1 cm/s, respectively. The equivalent elastic modulus (E') of a friction pair is calculated using Eq. (S2):

$$E' = 2/[(1-\nu_1^2)/E_1 + (1-\nu_2^2)/E_2] \quad (\text{S2})$$

where E and ν are the elastic modulus and Poisson ratio for the friction pair material, respectively.

The wear scar on ball was seen as the Hertz elastic deformation region of an equivalent ball suffer the load (1 N). The wear scar diameter of the ball ($d = 0.227 \text{ mm}$) can be described by Eq. (S3):

$$d/2 = (3RF/4E'')^{1/3} \quad (\text{S3})$$

Thus, the equivalent ball radius (R) can be given by Eq. (S4) [S6]:

$$R = E''d^3/6F \quad (\text{S4})$$

where d represents the diameter of the worn area on the ball ($d = 0.227 \text{ mm}$) and E'' is the reduced Young’s modulus of the contact materials, can be calculated using Eq. (S5):

$$E'' = 1/[(1-\nu_1^2)/E_1 + (1-\nu_2^2)/E_2] \quad (\text{S5})$$

Accordingly, the h_c is found to be 36.3 nm. This result indicates the existence of a fluid layer between the tribopairs. The lubrication regime can be classified by the ratio (λ) of the film thickness to the combined surface roughness given in Eq. (S6):

$$\lambda = h_c/(\sigma_1^2 + \sigma_2^2)^{0.5} \quad (\text{S6})$$

where σ_1 and σ_2 are the surface roughness of the worn area on the ball (14 nm) and coating (8 nm), respectively. The λ is approximately 2.3 for the lubricant in our test, indicating that during the low friction period, the lubrication regime for “colloidal solution” was located at the mixed lubrication regime [S7].

Figure S3 provides XRD patterns of TaN and VN. Both of them have the standard cubic NaCl-structure, but the difference is that VN has poor crystallinity. It also indicates that the tribological behaviors of VB TMNs in three-phase contact environment are independent of the crystallinity.

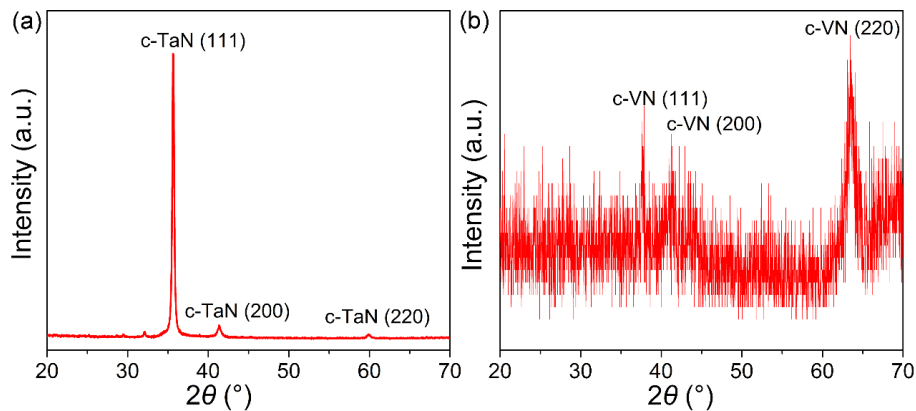


Fig. S3 XRD patterns for the (a) TaN and (b) VN.

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