

铜纳米颗粒改善润滑摩擦特性的机理研究

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摘要

铜纳米流体作为润滑剂可以有效降低摩擦系数, 改善摩擦副的形貌, 然而目前对其改善润滑摩擦的物理机制尚不清晰。本文采用分子动力学方法详细分析了凸峰剪切过程中, 铜纳米颗粒对摩擦副塑性变形、应力分布、摩擦力变化、以及摩擦副温度分布的影响规律, 得到了纳米铜颗粒改善润滑摩擦的物理机制。研究结果表明铜纳米颗粒受到凸峰的剪切作用形成了固体润滑膜, 阻碍了凸峰直接接触, 显著降低了黏着磨损, 有效地改善了摩擦副的应力分布, 显著降低了摩擦力和摩擦副的温度, 从而实现了抗磨减摩效果。

关键词

纳米颗粒, 凸峰, 分子动力学, 摩擦特性

Study on the Key Mechanisms of Lubrication and Friction Property Improvement by Copper Nanoparticle Characteristics

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Abstract

The mechanisms responsible for nanoparticles' antiwear and friction reduction properties are still not well known. Nanoparticles' improved effect on the rough surfaces contact is an important reason for the antiwear and friction reduction properties. The asperity shear is a typical way of rough surfaces contact. We performed molecular dynamics simulations to study the effect of copper (Cu) nanoparticles on the tribology properties of asperity shear. The friction pair is consisted by two

iron plates with asperities. The processes of asperity shear were given in detail. Because of the extrusion by the two asperities, the spherical Cu nanoparticle was transformed into a solid lubricating film, preventing the direct contact between the two asperities. Compared with the base fluid system, the stress distribution and surface wear of the nanofluid system were improved. During solid contact, the temperature of metal contact region and the friction force of the nanofluid system were lower than that of the base fluid system. Additionally, the height of the nanofluid system was increased by the presence of Cu nanoparticle, which helps to reduce the indentation depth of asperity and the probability of asperity contact.

Keywords

Nanoparticles, Asperity, Molecular Dynamics, Tribology Properties

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1. 引言

随着纳米技术的飞速发展，纳米颗粒在抗磨减摩领域的研究已经成为了热点。目前实验研究表明向润滑油中添加纳米颗粒可以有效地降低摩擦系数[1]，改善润滑同时提升燃油经济性[2]，还能强化换热并提高粘度和承载能力[3]-[5]。相对于传统的润滑油添加剂，纳米颗粒对温度的敏感度和摩擦化学反应降低[6]，其相较微米级和亚微米级颗粒具有最佳的润滑性能[7]。另外纳米颗粒尺度较小可以很好地通过过滤器[8]，渗透并沉积在摩擦表面形成摩擦膜[9][10]，能够有效降低摩擦和磨损[11]。因此，纳米颗粒在润滑油领域有着广阔的应用前景。

学者们相继提出了一些纳米颗粒改善润滑油性能的机理：(a) 滚珠机制[12]-[17]，(b) 隔离填充机制[18][19]，(c) 保护膜机制[20]-[24]，(d) 自修复机制[25]-[27]，(e) 剥落形成转移膜[28]。上述机理均是根据实验结果(磨损表面的 SEM 和 EDS 图像)进行推测得到的，缺乏理论支持；实验研究中往往同时包含边界润滑、薄膜润滑、流体润滑等多种润滑状态，无法针对某一特定润滑状态进行研究，得到的物理机制比较笼统；所以目前学者们对于纳米颗粒改善润滑摩擦机制的认识还比较模糊，这严重阻碍了纳米润滑油在实际中的应用，因而有必要对纳米颗粒改善润滑摩擦的机理进行细致研究。纳米颗粒改善粗糙表面间的接触是其提高润滑油抗磨减摩性能的原因之一。粗糙表面接触的形式大致可以分为三类：压痕、犁沟以及凸峰间的剪切(如图 1 所示)[29]，而凸峰间的剪切往往会产生大量的摩擦热，有可能导致润滑油膜的破裂、润滑油焦结以及摩擦表面黏着磨损，所以改善凸峰剪切时的摩擦特性显得尤为重要。实验研究发现金、钼、铜、镍等纳米颗粒都可以提高基础油的抗磨减摩性能[8][20][22][23][25][30]-[33]，尤其是对纳米铜颗粒的研究最多，这些金属的共性是晶格都属于面心立方晶格，且都属于软质金属，所以它们的润滑机理存在着共性。故本文将对球形纳米铜颗粒改善硬质凸峰(Fe)间剪切的机制进行研究。

纳米颗粒的尺度非常小，采用实验方法研究其改善凸峰剪切的机制是非常困难的，分子动力学方法能够从原子尺度上研究摩擦过程，并且可以针对特定的摩擦过程(凸峰剪切)进行研究，从而弥补实验研究的不足。目前大量的研究证明分子动力学方法可以很好地用于研究润滑摩擦机制，Zhong *et al.* [29]采用分子动力学方法研究了凸峰间的剪切过程，研究发现磨损过程与凸峰间的重叠度和键结强度有关。Peter *et al.* [34]从原子尺度上研究了粗糙表面的干摩擦过程，结果表明摩擦力随粗糙度的增加而增加，粗糙表面经过反复的摩擦后变得平坦。Lee *et al.* [35]研究了纳米小球的滚动摩擦过程，研究发现小球的尺寸和压

入深度影响着摩擦过程。Karthikeyan *et al.* [36]和 Lin *et al.* [37]研究了金属摩擦副滑动摩擦过程,得到了摩擦副塑性变形和微结构的演变过程。Zheng *et al.* [38]采用分子动力学方法研究了润滑剂碳链长度和载荷对粗糙表面固体接触的影响。Tamura *et al.* [39], Jabbarzadeh *et al.* [40]和 Berro *et al.* [41]采用分子动力学方法研究了传统润滑剂的润滑摩擦特性。然而,目前应用分子动力学方法研究纳米颗粒改善润滑摩擦机制的研究还很少。Lv *et al.* [42]采用分子动力学方法研究了 Cu-Ar 纳米流体的摩擦特性,主要分析了加载条件下纳米颗粒的运动行为,但并没有对纳米颗粒改善粗糙表面接触的物理机制进行详细研究。

综上,本文将采用分子动力学方法研究纳米铜颗粒改善凸峰间剪切的物理机制,着重分析添加纳米颗粒以后,模拟系统在摩擦力、高度以及凸峰接触时应力分布和温度分布上的变化情况,并根据模拟结果提出纳米颗粒改善润滑摩擦的机制。

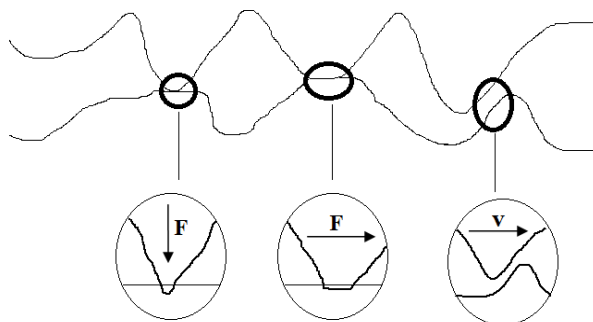


Figure 1. Schematics for three typical ways of rough surface contact
图 1. 粗糙壁面间 3 种典型接触方式的示意图

2. 物理模型和模拟细节

2.1. 物理模型

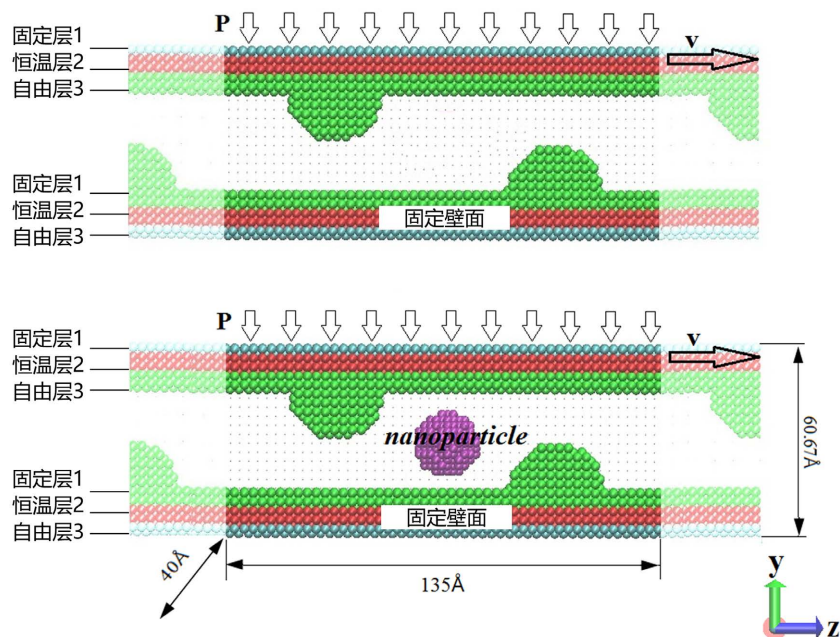


Figure 2. Snapshots of simulation models ($P = 0$ MPa). (a) Base fluid system and (b) nanofluid system
图 2. 物理模型($P = 0$ MPa)。(a) 基础流体, (b) 纳米流体

所有模拟均通过分子动力学的经典开源软件 LAMMPS [43]进行计算。模型由体心立方结构(BCC)的铁板和随机分布的液体流体组成,如图 2 所示。上下板共分为六层:固定层(1, 6)、恒温层(2, 5)、自由变形层(3, 4),其中恒温层的温度固定为 86 K。通过两个半径为 15 Å 的半圆柱体来构造两个板的凸峰。对于纳米流体模型,一个直径为 2 nm 的铜(Cu)颗粒被放置在两个凸峰之间。为了简化计算,本文选择液态氩(Ar)作为基础流体。法向载荷(P)缓慢施加在 z 方向,下板保持静止,上板沿 z 方向以速度 v 滑动。 x 和 z 方向上为周期性边界条件, y 方向为收缩边界条件,从而允许模拟时薄膜厚度波动。基础流体模型和纳米流体模型的原子总数分别为 18,529 和 18,786。

2.2. 势函数

非键结原子 Ar-Ar, Ar-Fe and Ar-Cu 之间采用 Lennard-Jones [44]势函数,原子间采用 Lorentz–Berthelot [45]混合原则计算 Ar-Fe and Ar-Cu 的势函数参数,具体为公式(1)至(3):

$$U(r_{ij}) = 4\varepsilon \left[\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^6 \right] \quad (1)$$

$$\varepsilon_{sl} = \sqrt{\varepsilon_{ss} \cdot \varepsilon_{ll}} \quad (2)$$

$$\sigma_{sl} = \frac{\sigma_{ss} + \sigma_{ll}}{2} \quad (3)$$

其中 ε 为势阱, σ 为原子间势能为零时的距离, r_{ij} 为原子间的距离。 s 和 l 分别代表固体和液体, Ar、Fe、Cu 之间采用的势函数具体数值如表 1 所示。

固体原子(Fe-Fe, Cu-Cu, Fe-Cu)之间采用嵌入原子势(EAM) [46]:

$$U = \sum_i F_i \left(\sum_{j \neq i} \rho_j(r_{ij}) \right) + \frac{1}{2} \sum_{j \neq i} \phi_{ij}(r_{ij}) \quad (4)$$

其中 F_i 为根据原子电子密度 ρ 确定的嵌入势能, ϕ 为作用势能, i 和 j 分别代表不同原子。具体 EAM 势参数参考 Bonny 等人[47]的研究。

Table 1. LJ potential parameters for simulation 38

表 1. LJ 势能参数[46]

	σ (Å)	ε (ev)
Ar-Ar	3.405	0.01042
Fe-Fe	2.321	0.52707
Cu-Cu	2.338	0.41016
Ar-Fe	2.863	0.0741
Ar-Cu	2.872	0.06536

2.3. 模拟细节

每次模拟由弛豫 400 ps、压缩 400 ps、再次弛豫 400 ps、剪切 1600 ps 四个步骤组成,在弛豫过程中,模拟温度设置为 86 K,确保低沸点的液体 Ar 始终保持液态。此后,对上板施加均匀分布的载荷 P 后再次运行一段时间使系统再次平衡。在此阶段,利用 Nose-Hoover 控温方法控制第 2 层和第 5 层原子的温度保持在 86 K。最后将上板沿 z 方向以速度 v 的匀速滑动。本文所用势函数的截止半径为 $2.5\sigma_{Ar}$,模拟时间步长为 0.002 ps,采用 Velocity-Verlet 算法求解运动方程。

摩擦力与面积 F_{fric} 定义为 $F_{fric} = F/A$ ，其中 F 和 A 分别代表上板沿运动方向稳定施加的力和面积。

3. 结果和讨论

3.1. 凸峰接触过程

上板载荷为 300 MPa，滑动速度为 10 m/s 时凸峰接触过程如图 3 所示。当滑动时间 $t = 1.5$ ns 时，纳米颗粒在两个凸峰间开始受到挤压，此时基础流体系统还未出现固体接触。在 $t = 1.9$ ns 时刻，由于纳米颗粒的存在，纳米流体系统已然形成了 Fe-Cu-Fe 的摩擦形式，纳米铜颗粒形成了固体润滑膜从而避免了凸峰间的直接接触，基础流体系统的两个凸峰则直接接触并出现了剪切效果。当滑动时间 $t = 2.0$ ns 时，纳米铜颗粒形成的固体润滑膜出现断裂，两个凸峰的原子间出现键结；对于基础流体系统，凸峰与基底间出现了晶格缺陷，这将使得摩擦表面容易出现磨损。当 $t = 2.12$ ns 时，两个模拟系统的凸峰原子间均出现了大面积的键结，基础流体系统还出现了材料迁移。当 $t = 2.24$ ns 时，两个凸峰分离，从图中可以看出两个系统均出现了磨损和塑性变形，并且基础流体系统的磨损情况较纳米流体系统严重，纳米铜颗粒受到挤压剪切后分离成两部分并分别紧密的附着在两个凸峰上，这是实验研究[22][23][33]在摩擦表面检测到铜单质的原因之一。

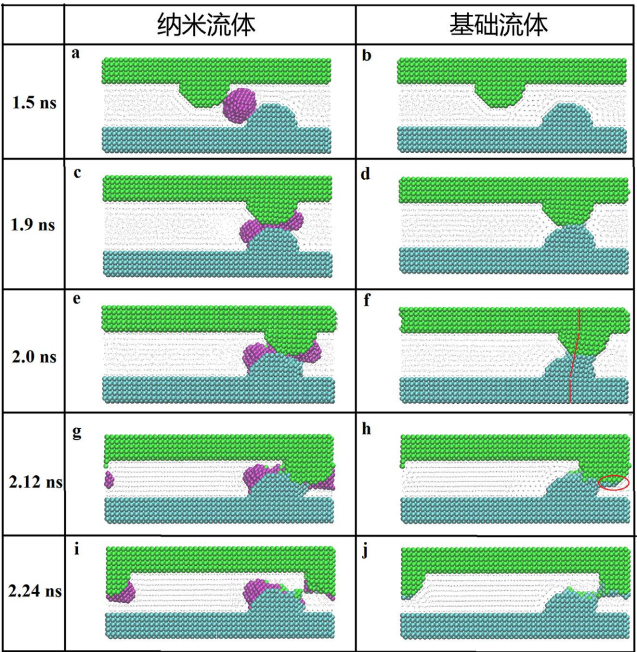


Figure 3. Process of asperity shear. To make the snapshots clear, the upper and lower plates are showed in different colors. $P = 300$ MPa, $v = 10$ m/s

图 3. 凸峰剪切过程。为了方便对比，上板和下板分别采用不同颜色。 $P = 300$ MPa， $v = 10$ m/s

图 4 所示为模拟系统的高度随时间的变化规律。当 $t = 1.5$ ns 时，纳米颗粒受到挤压的同时，纳米流体系统高度开始提高。当 $t = 1.76$ ns 时，基础流体系统的两个凸峰开始接触，系统的高度开始上升，而此时纳米流体系统的高度达到最高值。随着上板的滑动，两个系统高度达到最大值后接着开始下降并在 $t = 2.12$ ns 时达到最低点(如图 3g，图 3h 所示)。待两个凸峰脱离接触以后，系统高度重新上升。分析图 4 还可以发现纳米流体模拟系统的高度高于基础流体，尤其是当纳米颗粒受到挤压时(1.5 ns $< t < 2.12$ ns)的效果更加明显，这对于降低摩擦磨损是非常有利的。如图 5 所示，纳米铜颗粒使得系统的高度增加，也就降低了凸峰与摩擦表面接触的几率以及凸峰的压入深度，从而减少磨损降低摩擦力。

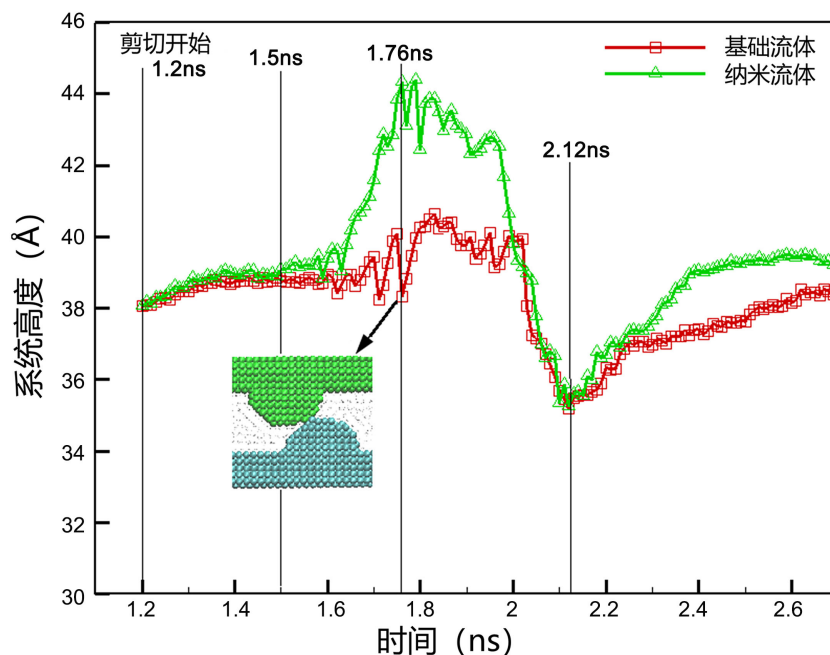


Figure 4. Time evolution of the height of systems. $P = 300 \text{ MPa}$, $v = 10 \text{ m/s}$

图 4. 模拟系统的高度随时间的变化规律。 $P = 300 \text{ MPa}$, $v = 10 \text{ m/s}$

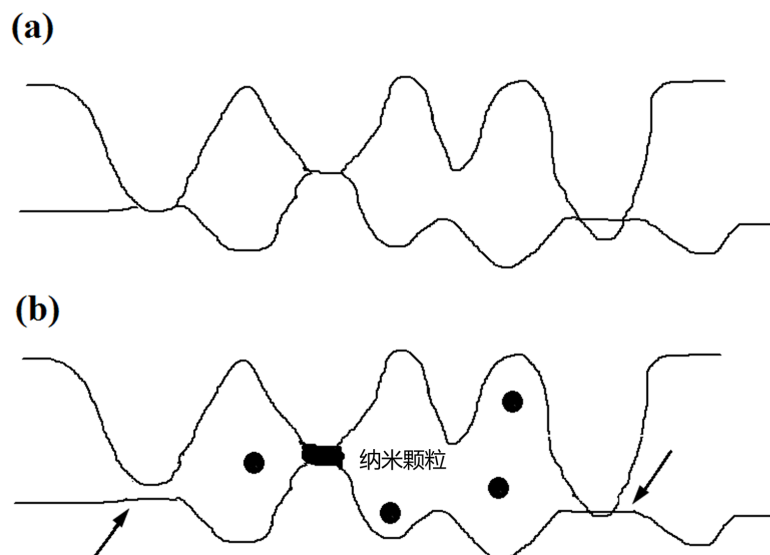


Figure 5. Mechanism of Cu nanoparticles for improving tribological properties. (a) State without nanoparticle and (b) state with nanoparticles

图 5. Cu 纳米颗粒改善润滑的物理机制。(a) 无纳米颗粒, (b) 有 Cu 纳米颗粒

图 6 所示为凸峰接触时原子的应力(Von Mises)分布情况, 图中所示时刻为 $t = 1.9 \text{ ns}$, 此时纳米铜颗粒受挤压所形成的固体薄膜还未断裂, 纳米流体系统凸峰间的摩擦形式为 Fe-Cu-Fe。如图所示最大应力值均分布在固体接触区域, 摩擦副的基底上也出现了应力集中的区域, 这说明凸峰的剪切作用容易导致材料内部发生位错, 进而可能发生疲劳磨损。对比两个图可以发现纳米铜颗粒所形成的润滑膜很好地改善了应力分布, 它不仅降低了凸峰的应力值, 还有效的缩小了基底上应力集中区域, 从而可以降低凸峰剪切过程所造成的磨损。

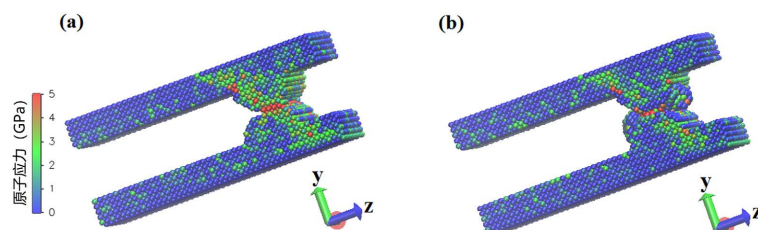


Figure 6. Atomic stress (Von Mises) of the solid atoms (Fe plates and Cu nanoparticle). (a) Base fluid system and (b) nanofluid system. $P = 300 \text{ MPa}$, $v = 10 \text{ m/s}$, shearing time $t = 1.9 \text{ ns}$

图 6. 凸峰(Fe-Cu)接触时原子的应力(Von Mises)分布。(a) 基础流体 (b) 纳米流体。 $P = 300 \text{ MPa}$, $v = 10 \text{ m/s}$, $t = 1.9 \text{ ns}$

3.2. 摩擦力

上板在滑动过程中会发生凸峰间的接触，摩擦力不可避免得会有较大幅度的变化。图 7 所示为摩擦力随滑动时间的变化情况。当纳米颗粒未受到挤压时($t < 1.5 \text{ ns}$)，基础流体和纳米流体的摩擦力非常接近。之后，纳米颗粒受到挤压，摩擦力升高，而基础流体的摩擦力仍保持较低值。当滑动时间 $t > 1.76 \text{ ns}$ 时，基础流体系统开始出现固体接触，摩擦力急剧上升并超过纳米流体系统。此时，纳米铜颗粒在凸峰间形成了固体润滑膜，纳米流体系统凸峰间的滑动主要集中在铜薄膜区域，而铜原子之间的作用力低于铁原子之间的作用力，所以纳米流体系统的摩擦力低于基础流体。对于纳米流体系统，当 $t = 2 \text{ ns}$ 时，纳米铜薄膜出现断裂，两个凸峰的原子直接接触，摩擦力急剧上升。如图 7 所示在椭圆位置处，两个系统的摩擦力急剧下降，这是因为上板的凸峰沿固体交界面向下滑行时，下板凸峰的部分原子会对上板凸峰产生斜向上的作用力 F ，水平方向的分力 F_1 推动上板向前滑行，另外下板凸峰还有部分原子会阻碍上板的滑行产生反向水平作用力 F_3 ， F_1 与 F_3 的合力仍然表现为阻碍上板滑行，所以图中摩擦力只是急剧下降但并没有变为负值。当纳米铜薄膜断裂以后，纳米流体系统的摩擦力仍然低于基础流体，这是因为在两个凸峰接触界面上仍然有铜原子分布，降低了凸峰间接触面积，从而降低了摩擦力。此外，在凸峰剪切过程中，摩擦力曲线呈锯齿状，说明产生了粘滑效应[48]，在纳米铜薄膜断裂之前，纳米流体系统的摩擦力呈稳定的周期性震荡，说明纳米铜颗粒所形成的薄膜可以很好地起到润滑效果。

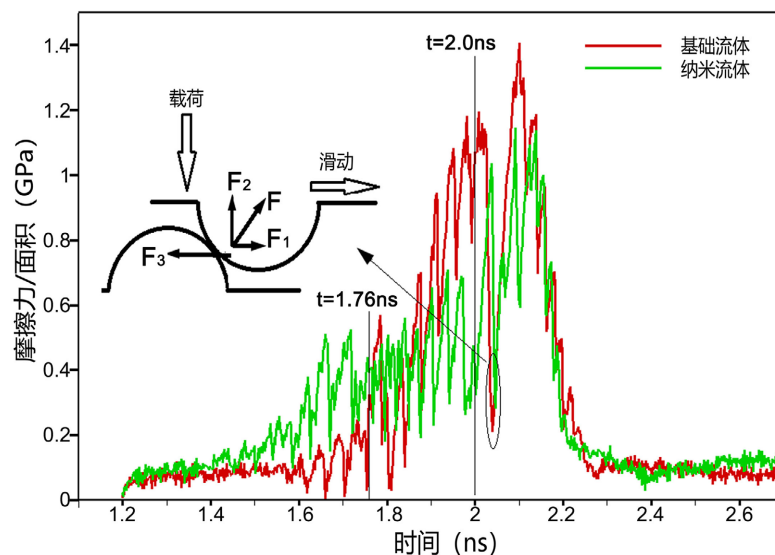


Figure 7. Friction force/area as a function of shearing time. $P = 300 \text{ MPa}$, $v = 10 \text{ m/s}$

图 7. 摩擦力随滑动时间的变化。 $P = 300 \text{ MPa}$, $v = 10 \text{ m/s}$

3.3. 温度变化

在凸峰剪切过程中会产生大量的摩擦热,使得固体接触表面的温度升高,而固体接触面的温度特性对于摩擦表面的相互作用和磨损影响很大,所以本文研究了凸峰剪切过程中固体区域的温度分布情况。当两个凸峰发生接触时,沿 y 方向将固体区域平均分成若干层,然后计算每一层的平均温度,从而得到温度分布曲线。图 8 所示为多个时刻的温度分布情况,从图中可以看出,任意时刻两个模拟系统温度最高区域均为 y 轴中间区域,即凸峰接触区域,纳米流体系统的温度以及 y 方向的温度梯度明显低于基础流体。当 $t = 2.04$ ns 时,基础流体系统的最高温度达到了 135 K,相对于热浴层的温度(86 K)提高了 57%。 $t = 2.08$ ns 时,纳米流体系统的最高温度为 104 K,只相对于热浴层温度提高了 21%。上述现象说明纳米颗粒通过形成固体润滑膜减少摩擦界面直接接触,抑制局部过热,可以有效降低固体接触区域的温度。较低的接触温度一方面延缓了润滑油在高温下的氧化与热分解过程,减少了焦化沉积物的生成;另一方面减弱了金属表面的塑性变形倾向与黏着磨损程度,避免了因高温导致的材料软化、剥落及界面剪切强度升高。此外,温度梯度的降低还减少了热应力集中对摩擦表面完整性的破坏。这将有助于防止润滑油结焦和降低摩擦表面磨损,从而提升润滑系统的长期稳定性和抗磨性能。

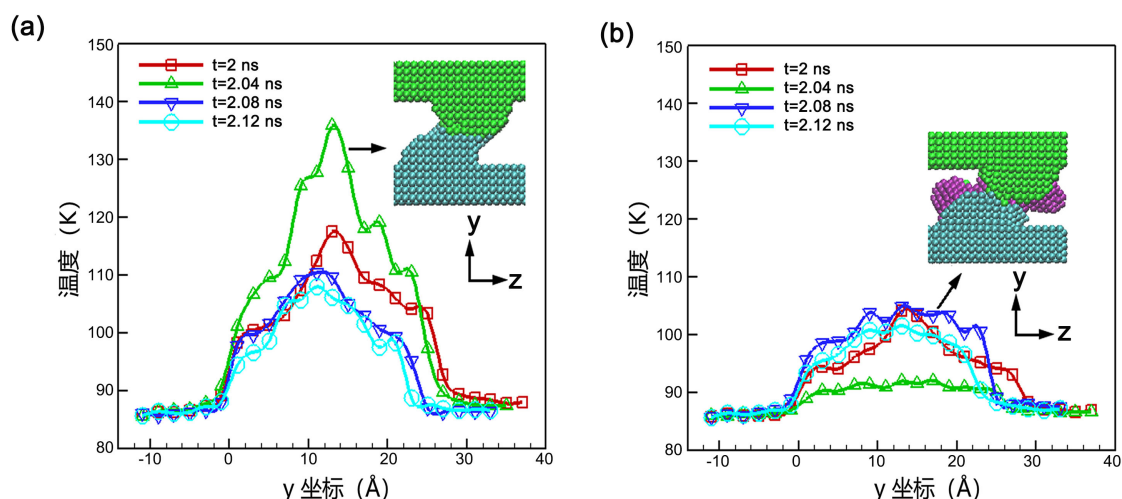


Figure 8. Temperature profiles of solid atoms along y dimension at different shearing times. (a) Base fluid system and (b) nanofluid system. $P = 300$ MPa, $v = 10$ m/s

图 8. 凸峰接触时的温度分布。(a) 基础流体 (b) 纳米流体。 $P = 300$ MPa, $v = 10$ m/s

4. 结论

为了研究纳米铜颗粒改善润滑摩擦的机制,本文采用分子动力学方法研究了凸峰剪切过程中纳米流体和基础流体摩擦特性的不同。文中主要分析了基础流体和纳米流体系统在系统高度、应力分布、摩擦力和温度分布上的不同,得到了如下结论:

(1) 在凸峰剪切过程中,纳米颗粒受到挤压剪切作用在两个凸峰间形成了固体润滑薄膜。这层润滑膜可以大大降低固体接触区域应力值改善材料内部应力分布,从而降低摩擦表面磨损。由于纳米颗粒的存在,纳米流体系统高度高于基础流体,也就降低了凸峰与摩擦表面接触的几率以及凸峰的压入深度,从而减少磨损降低摩擦力。

(2) 纳米铜颗粒形成薄膜可以很好的起到润滑作用,从而降低摩擦力。当铜薄膜断裂以后,由于两个凸峰接触界面上仍然有铜原子分布,纳米流体的摩擦力仍然低于基础流体。

(3) 纳米铜颗粒可以大大降低凸峰剪切时的温度,可有效地防止润滑油结焦和降低摩擦表面磨损。

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