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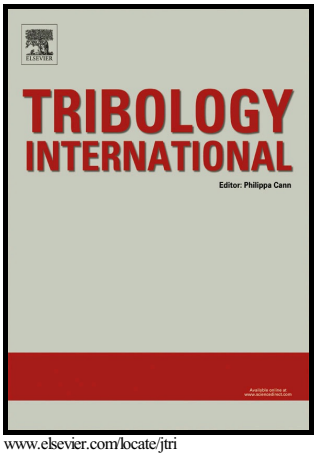

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The structural, tribological, and rheological dependency of thin hexadecane film confined between iron and iron oxide surfaces under sliding conditions

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Abstract

Molecular dynamics simulations have been carried out to investigate the tribological, structural and rheological properties of thin film hexadecane confined between different iron and iron oxide surfaces. The interfacial slip becomes severe with the increase of loading pressure and shear rate but it is insensitive to temperature. The shear stress increases with the loading pressure whereas the coefficient of friction shows a contrasting propensity. The shear stress and coefficient of friction increase with shear rate; and decrease with higher surface temperature. A logarithmic function has been proposed to correlate the variation of friction with shear rate. The shear viscosity increases exponentially with the loading pressure but this rheological component levels off when the loading pressure exceeds a critical value.

Keywords: molecular dynamics; thin film lubrication; hexadecane; iron oxide

Introduction

Alkanes have attracted numerous investigations in thin film lubrication because they possess desirable physical characteristics such as low friction [1], and high mechanical and thermal slip at the solid-fluid interfaces [2]. Experimental and theoretical investigations reveal the low adhesive strength of *n*-alkanes with metal and metal oxide surfaces due to their physisorption nature [3-5]. A wall-induced layering of thin *n*-hexadecane film has been