TRIBOCHEMICAL REACTION OF SODIUM POLYPHOSPHATE ON IRON OXIDE SURFACE IN METAL FORMING

M.H. Le[a*], A.K. Tieu[a], H.T. Zhu[a], D.T. Ta[a]
*mhl980@uowmail.edu.au
[a]School of Mechanical, Materials and Mechatronic Engineering, University of Wollongong, Northfield Avenue, Wollongong, NSW, 2522, Australia

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ABSTRACT
An appropriate lubricant is necessary in a hot metal manufacturing process due to negative effects at elevated temperature such as enormous friction, considerable wear and severe oxidation. Currently, zinc diakyldithiophosphate (ZDDP) is the most successful lubricant additive which can form an antiwear polyphosphate film on the interface between metallic surface and lubricant. In the effort of designing a new lubricant which can withstand high pressure and elevated temperature for hot rolling of steel, the studies of alkali polyphosphate have been conducted. With good antiwear property, friction reduction in harsh condition and being an environmentally friendly lubricant, inorganic polyphosphate glass is considered to be a candidate to replace ZDDP for high-temperature tribological applications [1]. In previous studies, the polyphosphate film has been observed after tribological process with layered structure and gradient composition. The digestion of iron oxide into polyphosphate film which shortens the polymer chain has been proven[2, 3]. Even though the experiment studies show some interesting properties of alkali polyphosphate boundary film on elevated temperature interface, the detailed mechanism between them is still unknown due to limitation of analytical method in severe conditions. In this study, a theoretical method has been carried out to understand the behavior of lubricant and surface interaction in atomistic scale.The chemical reaction and adsorption of lubricant on iron oxide surface has been performed on quantum calculation package Dmol^3 with periodic boundaries and GGA PBE functional.The configurations and energies obtained from the simulation have been validated with the experimental and theoretical works of phosphate adsorption on iron oxide surface. Besides literature pre-mentioned Fe-O-P linkage, direct Fe-P bond has been observed in the simulation which achieved as stable energy as the bond through bridging oxygen. The interaction between lubricant and surface through phosphorus or oxygen has proved to be an effective contribution of successful tribological role of alkali polyphosphate in reducing friction and wear.

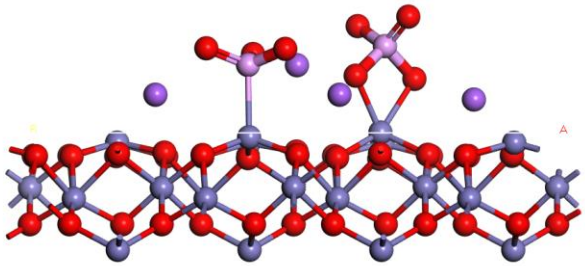

Fig.1 Fragments of tetrasodium pyrophosphate after P-O bond breaking adsorbed on iron oxide surface. The adopted color scheme is: P in pink, O in red, Fe in blue, and Na in purple.

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