MODELING OF ADHESION AND ADHESIVE WEAR: A COMPARISON BETWEEN ATOMISTIC AND CONTINUUM METHODS

E.M. Bortoleto [a*], R.M. Souza [b]
*eleir.bortoleto@itv.org
[a] Instituto Tecnológico Vale,
35400-000, Ouro Preto, Minas Gerais, Brazil
[b] University of São Paulo - Department of Mechanical Engineering
05508-030, São Paulo, SP, Brazil

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INTRODUCTION

This work presents a comparative study between molecular dynamics (MD) and finite element method (FEM) models of the unidirectional contact between a two-dimensional plane-strain square (indenter) and a flat slab, in order to evaluate adhesive contact and adhesive wear. The FEM models were based on the previous work by Bortoleto et al. [1], who analyzed different pairs of materials and their adhesion intensity by calculating surface attractive forces in terms of the Lennard-Jones interatomic potential and Hamaker constants. The MD models reproduced the same geometry used in the previous FEM models in order to allow the correlation between the atomistic MD numerical modeling results and the cases analyzed by the continuum mechanics using FEM. The results reveal that there is a qualitative correlation between the amounts of material transferred between the surfaces as calculated in the two numerical approaches. This indicates that the FEM adhesion models [1] could reproduce phenomena that previously required atomistic approaches.

MATERIAL AND METHODS

A finite element analysis was conducted to investigate the contact problem of a linear elastic square punch indenting an elastic-plastic deformable slab. Different arrangement of surface pairs were evaluated, by combining cooper, aluminum and iron surfaces. An *ad hoc* user FORTRAN subroutine designed to calculate the adhesion forces was coupled to finite element solver Abaqus. Adhesion forces were introduced in the system as forces acting on the surfaces as a function of the separation distance between the surfaces.

Regarding MD models, interactions between atoms in all simulations were described by the embedded atom method (EAM) potentials for cooper, aluminum and iron surfaces.

For both MD and FEM analyses, approximation and separation steps were modeled. During the separation step, material transfer between surfaces can occurs due to adhesion with respect to damage initiation and propagation at the flat slab. The parameters considered in the simulations included normal load, chemical affinity, and system size.

RESULTS AND DISCUSSIONS

Wear related to adhesion phenomena in dry contacts was estimated based on the amount of material transfer from the slab to the indenter, evaluating this transfer for each of 24 different combinations of surface pairs and contact conditions. An adhesive wear map, based on an equation that correlates the material parameters and material loss due to adhesion, was proposed. The results indicate that the chemical affinity between bodies in contact is more related to adhesion than the applied load. The amounts of material transferred between the surfaces as calculated by FEM models is correlated with the results of MD models (Fig. 1), which indicates that the proposed FEM adhesion models were able to reproduce atomistic phenomena.

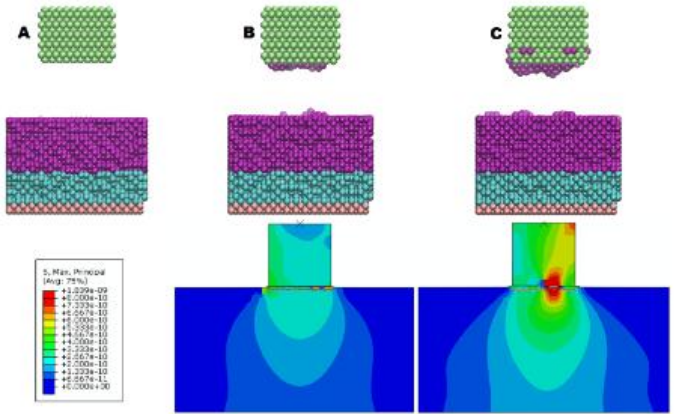

Fig.1 Comparison between MD (top) and FEM (bottom) analyzes showing the contact sequence (copper surfaces): initial touch (A) and penetration of 1 (B) and 2 (C) atomic layers.

REFERENCES

[1] Bortoleto, E.M., Prados, E.F., Seriacopi, V. et al. Friction (2016) 4: 217. https://doi.org/10.1007/s40544-016-0119-5