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ScienceDirect

Procedia Engineering 150 (2016) 435 – 441

Procedia Engineering

www.elsevier.com/locate/procedia

International Conference on Industrial Engineering, ICIE 2016

Studying the Resonance Processes in the Surface Layers of Friction Pairs with Lubrication by Means of Molecular Dynamics

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Abstract

The article investigates the resonances of diffusion processes using molecular dynamics method (MD) for heat-resistant steel carbonitriding. For this purpose, three types of resonances processes are used, different in terms of influence of thermal shock (TS) in the surface layers of heat-resistant steel with carbonitriding coating. The first type is nonlinear (cubic) resonance based on the frequencies of atomic fluctuations, ω_0 in crystal lattice α-*Fe* and frequency under force of TS, ω. The second type is associated with resonance harmonics $\omega(i)$ force of TS and spectrum of atomic fluctuations in the lattice. The third type is related to the damping law of attenuation resonance processes in the depth of the surface. The article explores the first type of resonance processes. The result of resonance process conduction in the surface layer occurring to phase structural transformation reduces the formation of secondary structures, which determine the performance properties of the friction pairs.

Peer-review under responsibility of the organizing committee of ICIE 2016

Keywords: the resonance mechanism of diffusion; the method of molecular dynamics; thermal shock; secondary structures; structural phase transitions; sliding friction with lubrication.

1. Introduction

During friction, in the surface layers of friction pairs occurs structural-phase transformations leading to the formation of secondary structures which determine the operational properties of friction pairs such as the propensity to grasp, associated with a sharp increase of the local friction factors [1]. The formation of secondary structure is associated with diffusion and diffusion-free (polymorphic) processes in the surface layers. A significant increase in the diffusion coefficient (D = 10^{-5} - 10^{-8} m^2/s) was established experimentally. This phenomenon is determined:

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Peer-review under responsibility of the organizing committee of ICIE 2016
doi:10.1016/j.proeng.2016.07.011

firstly, by the morphology of the frictional surfaces in the form of sub- and micro-roughness during friction process to the appearance of the pulsating thermal processes (thermal cycling) [2]; secondly, as a result of thermal cycling occurring to thermal shocks (TS) and the related increase in pressure P at the surface zone [3]. Thus, it is in this context, there is a necessity for research into the mechanisms of diffusion, as the widely used diffusion mechanisms (vacancy, exchange, etc.) could not be exploited to explain the sharp increase in the diffusion coefficients.

Recently, methods of molecular dynamics (MD) have been used for the study of diffusion processes which allow to study these processes through simulation, which has its own characteristics. If during simulation the nuclear lattice and electrons are partially neglected and only the volumetric phenomena (the continuum) is considered, then in the simulation of diffusion processes it is preferable to consider the processes at the level of the crystal lattice. Since conclusions about the mechanisms of diffusion should be done on the basis of the energy estimation and the controlling process, it is necessary to set the binding energy between atoms in the form of potentials of pair interactions (PPI). The presence of PPI raises the possibility of formation of a crystallite with a given set of properties with the given number of atoms N (usually $N \leq 10^5$). Therefore, the oscillatory processes are considered in the simulation since the wave processes occur in the metal when $N \geq 10^6$ [4].

In the works [5, 6] is presented the results of simulations MMD about the movement process of atoms under the influence of TS in the surface zone of complex alloy heat resistant 25Kh3M3NBTsA. The analysis of trajectories of movements of atoms has allowed to define the diffusion mechanism as cooperative (relay) with diffusion coefficients $D = 10^{-6}$ - 10^{-8} м^2/s. However, to explain the higher experimental diffusion coefficients in the order of $D = 10^{-5}$ м^2/s, this mechanism is not possible. Preliminary estimates showed that another mechanism may occur under the influence of TS defined as resonance. This assumption is based on the possibility of matching the frequency (ω_0), vibrations of the atoms in the crystal lattice vibration frequencies (ω), and external force (TS).

Experiments have revealed the presence of crystals in the zones with abnormally high amplitudes of the vibrations of the atoms without external influence. The theoretical justification of this phenomenon was given by M. Born [7]. The presence of impurities and defects in the crystal affects the spectrum of vibrations of atoms due to the appearance of oscillations, called localized modes. For sufficiently large distortions of the lattice can occur in resonant modes, resulting in micro-volume resonances. In [8], where they studied lattices with strong anharmonic state and took into account collective phenomena in phonon subsystem, it is established that as a result of nonlinear resonance and synchronization occurs the phonon frequencies. These processes lead to structural instability of the lattice, martensitic transformations and melting.

2. Formulation of problem

Resonant processes during friction are fast ($\tau \approx 10^{-12}$ s). In this regard, the modelling of these processes is obviously preferable. In the simulation the resonance is defined as a sharp increase in the amplitudes of the forced vibrations of N atoms, arranged in a set of lattices representing the imaginary crystallite. The atoms undergo thermal vibrations with frequencies ω_0 and subjected to external periodic effects (TS) with the frequency ω. According to Born-Lederman theory the frequency distribution of fluctuations of the real metal, presented in the form of a large lattice of N atoms approximately coincides with the distribution of imaginary frequencies of the lattice with cyclic boundary conditions [7]. In turn, an imaginary system of N atoms is completely equivalent to a chain of simple harmonic oscillators with corresponding frequencies ω_0^i. If this chain link PPI, in the language of the theory of vibrations the motion of atoms in the chain is defined as the movement of the oscillators in the field, given PPI [9]. In the absence of external effects (TS) such a system is mathematically described as autonomous. Since the crystal lattice has PPI rigidity, its fluctuations are dissipative. If the decomposition of the PPI members consider the 3rd order, i.e. thermal anharmonicity, then, first of all, the system will be nonlinear (cubic), and, secondly, there are the dispersion of the frequency (spectrum), as the anharmonic members provide a link between normal lattice vibrations. If we consider the anharmonic terms, the terms of higher order play essentially the role of viscous medium, dissipating the energy dispersion of the oscillators. In the presence of TS system becomes a non-autonomous cubic nonlinear dissipation and dispersion. The mathematical description of such a system is given by [9]: