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# ATOMISTIC SIMULATION OF SURFACE CYCLIC SLIP IRREVERSIBILITY IN FCC METALS

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**Summary** The mechanical behaviour of surface steps created by the emergence at the free surface of gliding dislocations, subjected to cyclic loading is examined using molecular dynamics simulations. Different face centred cubic metals, Al, Cu, Ag and Ni are analysed. An atomistic reconstruction phenomenon is observed at these surface steps which can induce strong irreversibility. The irreversibility cumulates and a micro-notch is produced whose depth increases cyclically. A rough estimation of surface irreversibility for pure edge dislocations gives an irreversibility fraction between 0.5 and 0.75 in copper. An analysis coupling surface mechanisms with the classical EGM bulk slip irreversibility model gives an irreversibility fraction of 0.62 in copper for pure screw dislocations, contrary to many sketches proposed in the past. It seems that oxygen molecules cannot lead to higher irreversibility as they have no major influence on different mechanisms linked to surface relief evolution.

## INTRODUCTION AND SIMULATION TECHNIQUES

Fatigue is one of the major damage mechanisms of metals. Fatigue damage generally starts at free surfaces from the accumulation of unreversed slip steps. And cyclic micro-plasticity based on the glide of dislocations is one of the mechanisms responsible for the fatigue phenomena in single phase fcc metals and alloys. The slip irreversibility can be characterized by the fraction  $p$  of irreversible plastic shear strain per cycle compared to the total plastic shear strain ( $p = \Delta\gamma_{\text{plirr}} / \Delta\gamma_{\text{pl}}$ ). The EGM II model describes the evolution of the surface roughness based on the dislocation production and annihilation in the bulk [1]. This EGM model only considers bulk mechanisms and neglects the surface slips mechanisms and environment effect. The aim of this work is to evaluate random surface step irreversibility by atomistic analyses of surface step evolution mechanisms in order to complete the EGM (part II) model by explicitly taking into account the mechanics of surface steps.  $b = a\sqrt{110}/2$  edge dislocations are inserted in the bulk and then glide to free surfaces and create surface steps. Molecular dynamics simulations are carried out in this work to follow the atom movements from the very first steps created at a free surface until their accumulation, and from the very first cycle to several cycles.

N-body embedded atom model (EAM) like potentials are used for simulations in vacuum. ReaxFF (reactive force field) potentials are used for simulations in oxygen environment. All these potentials give fairly correct estimations of different physical properties of the materials analyzed. The crystallographic orientations of the three axes are x: [-131], y: [714] and z: [11-2]. Contraction-dilation (compression/extension) cycles will be applied along the y: [714] direction. This choice of orientations has several advantages: it corresponds to a large Schmid factor value equal to 0.445, it makes the slip plane and the surface steps easy to visualize, and it is oriented for single slip in agreement with older studies. There are nearly 12,500 atoms in the box and periodic boundary condition is used along the z-direction. The time step used in the simulations with EAM potentials and ReaxFF potentials are respectively 1 fs and 0.5 fs, small enough to ensure its stability.

## MAIN RESULTS

A surface step reconstruction phenomenon is observed when an inserted dislocation glides out of the surface and creates a surface step. The geometry of the surface step changes afterwards. Some atoms on the surface step 'fall' down to the lower surface as illustrated by arrows in Figs 1a and 1b, the atoms of the column position M will move to N and the concave shape of the surface step thus turns into a convex geometry. By doing this move, the step atoms get more neighbours, optimize their cohesive energies and thus minimize the surface step energy. This phenomenon is observed for all geometries of surface steps. Three different types of mechanisms can be identified for the reconstruction depending on both the nature of the step and the temperature: the quasi-instantaneous reconstruction which occurs at all temperature in only a few picoseconds in case of larger surface steps, the thermal vibration assisted reconstruction whose rate depends on temperature and time, the surface diffusion assisted reconstruction which only takes place at higher temperatures and requires surface atomic diffusion and longer time, in the order of magnitude of 0.1 nanoseconds. The reconstruction can be achieved via just one mechanism or by the combination of two or three mechanisms. At room temperature, nearly all steps reconstruct, but at lower temperatures, non-reconstructed steps exist.

Reversibility of created surface steps are analyzed during opposite loading cycle and one full loading cycle is thus achieved. It is observed that when there is no arrival of opposite sign dislocations during the opposite loading, previously created and not reconstructed surface steps can be reversible although a critical resolved shear stress larger than one GPa is

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required for the reversion. This value is much larger than the usual stresses applied during experimental cyclic loadings which are only from several to hundreds of MPa. If the previously created steps are reconstructed, they are not reversible, even under a shear stress of at least 2GPa or more. When there are arrivals of opposite sign dislocations located in direct neighbor plane with respect to the previous dislocations, it is obvious that non-reconstructed surface steps can be erased. A reconstructed step cannot be fully erased by an opposite sign dislocation at low temperature and there is a remaining surface hole defect. Yet, if the temperature is high enough and the ‘surface diffusion activated reconstruction’ can take place, diffusing surface atoms can eventually fill the small hole of the surface and the step is finally completely erased. It is possible of course that opposite sign dislocations do not appear at immediate neighbouring planes. Simulations are thus carried out for cases where there is one, two, three or four atomic planes between the planes of insertion of the opposite sign dislocations. It is observed that in these cases, surface steps cannot be fully erased and a micro-notch is initiated and grows deeper cycle by cycle, as shown in Figs. 1c.

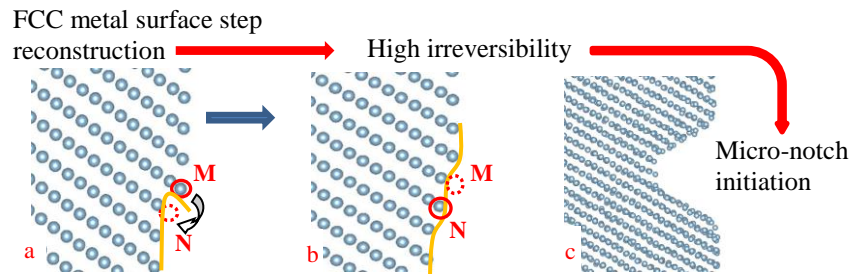


Fig.1. Surface step reconstruction (a, b) and micro notch initiation (c) in Al at 300K. Mechanisms are the same in Cu, Ag and Ni.

Similar simulations are carried out in oxygen environment. Oxygen molecules are adsorbed on metal surface and dissociate into oxygen atoms which are absorbed. This locally generates high-temperature areas. The temperature and the oxygen gas pressure have effects on the surface oxygen diffusion depth. Yet, probably because oxygen atoms are very lightweight compared to metal atoms, absorption of oxygen has no significant effect on the surface step reconstruction and does not impede the gliding of dislocations towards the surface as shown in Figs. 2. Oxygen will thus not increase the step irreversibility and has no major effect on the surface roughness. This holds only for surface relief evolution and agrees with experimental observations [3].

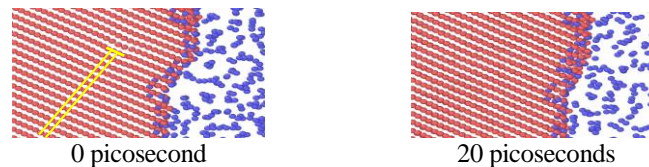


Fig.2. Oxygen effect for the gliding of dislocations towards the surface at 300K in Ni.

## DISCUSSIONS

The atomistic simulations carried out in this work show a strong irreversibility of surface slips. A simple estimation of the irreversibility gives an irreversibility fraction between 0.5 and 0.75 in copper for pure edge dislocations and this value is 0.62 for screw dislocations combining bulk and surface mechanisms. The value of  $p$  that we evaluated is much larger than the value estimated by the EGM II model where a value of 0.4 was found considering pure screw dislocations, and even smaller for edge dislocations. Our value is much closer to the experimental AFM carried out on nickel in air where  $p$  is about 0.8 [2].

The irreversibility factor  $p$  estimated in this MD study in inert environment is almost at its maximum value and it is observed that oxygen environment does not increase surface irreversibility in nickel and copper. This is indeed in agreement with observations made by several workers who found that the PSB surface relief is the same for fatigue in inert environment and in air [3]. This shows that old sketches proposed in literature concerning effect of adsorbed atoms on slip irreversibility [4] are not valid for Ni and oxygen. Two more questions remains: how is surface slip irreversibility affected as surface crystalline oxide film is formed and how may we explain the large effects of environment on cyclic propagation [4]. Computations are in progress for answering questions.

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