FATIGUE AND ASSOCIATED MICROSTRUCTURAL ASPECTS

Atomistically based multiscale modelling

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Abstract. Quantitative atomistic modelling of annihilation of screw dislocations of opposite sign leads to a semi-quantitative account of the slip lines causing fatigue damage in ductile materials. In general terms this new result completes an experimentally assisted multiscale modelling approach and reconciles the basic yielding and exhaustion theories of fatigue.

1. Introduction

The repeated plastic strains sufficient to cause fatigue fracture are surprisingly small. Nevertheless, fatigue is clearly recognized as a multiscale phenomenon in plasticity. The Basinskis [1] have developed a quantitative observational picture of the macroscopic, microstructural and atomic levels of fatigue processes in face-centred cubic materials. Their general conclusion is that fatigue in fcc materials is an as yet unknown thermally activated process limiting the dislocation density during the prominent stage of "saturation" over large cumulative plastic strains and at temperatures ranging from about half the absolute melting temperature to near zero.

It is widely agreed that experimental and theoretical studies of fatigue at its different length scales require branches of materials research so different that collaboration becomes the key to progress. In the present short introduction to fatigue the focus is on the interplay of materials science and -physics: composite models of microstructures [2,3] must be connected to the discrete levels of dislocation plasticity. At these levels cross-slip processes are particularly interesting, partly because cross-slip appears to be the irreversibility generating the metastable dislocation microstructures responsible for fatigue [3-11]. Computer simulation of dislocation self-organization processes [12,13] have recently confirmed this crucial role of cross-slip.

However, continuum elastic dislocation modelling of fatigue must in the end be connected to atomic theory, otherwise it is without foundation, e.g. [14-16]. According to cross-slip theories of fatigue the length scales of the fatigue induced microstructures are governed by annihilation of opposite screw dislocations by cross-slip. This process has recently been modelled quantitatively at the atomic level by Rasmussen et al. [16],
so the following discussion is a first attempt to employ these atomic-scale result in multiscale modelling of fatigue. In particular it is of interest to see the quantitative implications of the idea that cyclic saturation in fatigue is associated with mutual annihilation of opposite jog-free screw dislocations.

2. Experiments, phenomenology and mapping of mechanisms

Materials for engineering design must resist fluctuating stresses and strains of different amplitudes, in different directions, at different temperatures and often under simultaneous attack from corrosion and radiation. In industrial materials fatigue depends on polycrystallinity and complicated chemical compositions. The effects of polycrystallinity involve parameters like the sizes, shapes and orientations of individual grains, while effects of chemical composition involve a transition from "wavy" slip at high cross-slip frequency to "planar" slip occurring at an (apparently) much lower cross-slip frequency.

![Figure 1. Hysteresis loop for polycrystalline Cu-30%Zn. A small asymmetry about the zero stress line is neglected to define the phenomenological "friction stress" and "back stress". From [21].](image)

2.1. EXPERIMENTS

The development of an understanding of the mechanisms of fatigue has required carefully controlled experiments on well-characterized model systems. In the simplest and most widely used type of control (e.g. Fig. 1) the material is strained cyclically in tension-compression at constant values of the plastic strain amplitude and temperature. Numerous studies of fatigue involve such experiments on single crystals of copper,