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Research paper

Mechanical properties of hydroxyapatite single crystals from nanoindentation data

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ABSTRACT

In this paper we compute elastoplastic properties of hydroxyapatite single crystals from nanoindentation data using a two-step algorithm. In the first step the yield stress is obtained using hardness and Young's modulus data, followed by the computation of the flow parameters. The computational approach is first validated with data from the existing literature. It is observed that hydroxyapatite single crystals exhibit anisotropic mechanical response with a lower yield stress along the [1010] crystallographic direction compared to the [0001] direction. Both work hardening rate and work hardening exponent are found to be higher for indentation along the [0001] crystallographic direction. The stress–strain curves extracted here could be used for developing constitutive models for hydroxyapatite single crystals.

1. Introduction

Bone is a composite material with an organic matrix and inorganic minerals arranged in a hierarchy of structures spanning several length scales (Mann, 1993; Currey, 2005). At the nanometer length scale, e.g., the structure consists of self-assembled collagen fibrils and inorganic hydroxyapatite nano-crystals (Elliott, 1994, 2002). The mechanical properties of the organic and inorganic phases together with their hierarchical arrangement impart bone its characteristic strength and toughness. There is therefore much interest in characterizing the mechanical properties of hydroxyapatite, not only for its importance in the overall mechanical behavior of bone in disease and in health but also for its wide-scale application in biomaterials, regenerated hard tissue, and in medicine (Rodrigues et al., 2003; Motskin et al., 2009). For instance, hydroxyapatite crystals act as an important reservoir for hosting different ions and cations and therefore play a key role in metabolic activity of the bone (Bazin et al., 2009). Recent research has shown that hydroxyapatite crystals may induce cytotoxicity and apoptosis of certain cancer cells (Hou et al., 2009).

Defects such as dislocation and their density play an important role in the bioactivity of hydroxyapatite crystals. Dislocations have a major influence on the processes that leads to bone apposition on bioactive materials. Dislocations also have an important role in *in vivo* dissolution processes and in crystal maturation of biological apatites (Porter et al., 2004). Dislocations allow plastic deformation through slip. Early studies using microscale compression tests along different

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