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Experimental and computational studies of ultrasound wave propagation in hexagonal close-packed polycrystals for texture detection

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Abstract

Texture in hexagonal close-packed (hcp) polycrystalline metals, often developed during thermomechanical processing, affects ultrasonic wave velocity. In this study, the relationship between bulk texture and ultrasonic wave velocity in aggregates of (predominantly) hcp grains is investigated using theoretical, numerical and experimental methods. A representative volume element methodology is presented, enabling the effects of texture on ultrasonic wave speed to be investigated in two-phase polycrystals, and is employed to examine the ultrasonic response of random polycrystals, textured polycrystals and macro-zones often observed in titanium alloys. Numerical results show that ultrasonic wave speed varies progressively with changing texture, over a range of $\sim$200 m s^{-1}, within bounds set by the two extreme single-crystal orientations. Experimental ultrasound studies and full electron backscatter diffraction (EBSD) characterization are conducted on unidirectionally rolled and cross-rolled Ti–6Al–4V samples in three orthogonal directions. In addition, the EBSD-determined textures are incorporated within the polycrystal model and predicted ultrasonic velocities compared directly with ultrasonic experiments. Good quantitative agreement is obtained and both the experimental and computed results demonstrate that ultrasonic velocity profiles exist for random, unidirectionally rolled and cross-rolled textures. The combined results indicate the possibility of the development of a methodology for bulk texture determination within Ti polycrystal components using ultrasound.

Keywords: Hcp polycrystal; Ultrasound; Texture; Macro-zones; EBSD

1. Introduction

Hexagonal close-packed (hcp) metals, particularly titanium, zirconium and magnesium, are key materials in the aero, nuclear and auto industries. For example, Ti–6Al–4V is employed extensively in aero-engine components and Zircaloy has been selected as the key material for cladding nuclear reactor fuels [1,2]. Often, the commercially useful metals are two-phase alloys (for example Ti–6Al–4V), comprising both hcp (alpha) and body-centred cubic (bcc) (beta) phases, which have differing elastic (and hence ultrasonic) responses [3]. At the single crystal level, both hcp and bcc materials are anisotropic elastically [4], which often results in properties at the macro- or component level, which are also highly anisotropic, depending upon the nature of the distribution of crystallographic orientations. The latter, known as texture, is highly relevant in determining component properties and performance.

The texture of an hcp polycrystal may be described in terms of at least three well-established techniques: pole figures, which are stereographic projections of relevant plane normals to show the distribution of orientations throughout the polycrystal; orientation distribution functions (ODFs), which are probabilistic distribution functions to depict the occurrence possibilities of orientations on

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relevant planes and directions [5]; and Kearn's factors, which consist of three factors describing the proportions of hcp crystals whose basal poles are aligned in the same direction as the three sample axes, e.g. the rolling, transverse and normal axes, respectively [6,7].

In addition to texture, for titanium products, there is another important factor that has significant impact on their mechanical properties; that is, the occurrence of macro-zones, which are regions of near-uniform crystallographic orientation, up to 100 times the size of a typical grain, observed in forged disks as well as in billets [8,9]. Research shows that the presence of macro-zones, where the local basal poles are aligned close to the loading direction, are responsible for crack nucleation and growth, and can drastically reduce component fatigue life [10,11]. Given the importance of texture and macro-zone defects in hcp materials, a non-destructive technique which enables their detection in three dimensions is of major significance. Indeed, recently, Moreau et al. [12] have presented a study of combined electron backscatter diffraction (EBSD) and ultrasonic techniques for the detection of macro-zones, which have provided, for the first time, experimental evidence that a macro-zone of known surface location can be identified with use of ultrasound, and that the ultrasonic interpretation has been validated by EBSD.

A number of methods are commonly used for texture evaluation, but they all suffer from being destructive in nature and feasible in a practical capacity for very small material volumes only. Recent X-ray diffraction methods [13,14], for example, enable three-dimensional (3-D) texture determination, though only destructively and within small material volumes, and at relatively high cost. EBSD, however, has achieved rapid acceptance in the field of metallurgy during the past 20 years and provides the most widely used technique for texture analyses, though it is confined to (mainly small) two-dimensional surfaces and remains destructive [15–18]. High-resolution EBSD has been pioneered by Wilkinson et al. [19], which in addition to texture detection, enables local strain measurement and the extraction of lattice curvature and density of geometrically necessary dislocations. These techniques are accurate and effective, but they are not suitable for non-destructive bulk texture evaluation.

Non-destructive evaluation (NDE) techniques have been under development as an alternative to microscopy for many years, with the majority using ultrasonic waves. One major branch of ultrasonic evaluation is the Rayleigh wave technique. The Rayleigh wave was widely used to detect cracks on surfaces [20,21], and has since found application in the analysis of surface texture [22–24]. However, as Rayleigh waves are constrained to be near the surface in a very thin layer with the depth of approximately a wavelength, they cannot be used for bulk texture evaluation.

Ultrasonic techniques have been developed to an advanced level for the NDE of defects internally located in solid components, including for cases of textured materials. However, the usual interest is to detect defects without the influence of the texture. For example, Chassignole et al. [25] employed an ultrasonic method to characterize the average elastic constants and grain orientations of austenitic stainless steel welds, which consist of coarse anisotropic crystals, but their major concern was restricted to weld inspection instead of texture evaluation. Moreover, the successful evaluation of grain orientations in coarse weld crystals could also be regarded as a demonstration of the applicability of ultrasonic methods in texture determination.

The use of ultrasonic techniques to examine texture has so far received less attention, but research can be categorized into two types: namely, ultrasonic attenuation and backscattering, and ultrasonic wave velocity methods. Han and Thompson [26] proposed a theory to predict backscattering coefficients in duplex microtextures consisting of macrograins and applied it to titanium alloys, and Yang et al. [27] introduced a model to study scattering-induced attenuation and used it to study micro-textured regions (MTRs, which have some similarities to macro-zones) and found good agreement between the prediction of the model and experimental results. The wave velocity method [28,29] involves constructing equations to describe the wave propagation of both longitudinal and shear waves in anisotropic polycrystals. Palanichamy et al. [30] studied the dependence of ultrasonic velocity on grain size in austenitic stainless steel, and found the velocity decreased with the grain size. The angular dependency of ultrasonic waves in hcp aggregates has been reported by Sayers [31], and provides experimental reference for the study presented in this paper.

In this study, dynamic crystal elasticity techniques are developed with microstructural model representations of single- and polycrystals, in both single- and two-phase hcp materials. Firstly, model Zr single-phase polycrystals with a range of textures are developed and their responses to ultrasonic excitation representative of laboratory testing techniques examined in order to demonstrate the strong variations in ultrasonic wave speed resulting from texture change, and the incorporation of a macro-zone. Next, laboratory-based ultrasonic scans and EBSD investigations are performed on two differing (unidirectionally rolled and cross-rolled) two-phase Ti samples, in which the ultrasonic responses and EBSD characterizations in three orthogonal directions are investigated. The EBSD characterizations, detailing both the hcp alpha and bcc beta phase crystallographic orientations and their distributions are then employed to construct representative model polycrystals with which computational ultrasound studies are then carried out in the three orthogonal directions. The model ultrasonic wave speeds are compared in detail with those determined experimentally in order to assess the feasibility of ultrasonics for texture measurement.

In the next section, ultrasound behaviour in anisotropic materials is briefly reviewed, followed by the development of dynamic elastically anisotropic finite element polycrystal