A NEW METHOD TO DETERMINE SINGLE CRYSTAL ELASTIC BEHAVIOR FROM POLYCRYSTALS

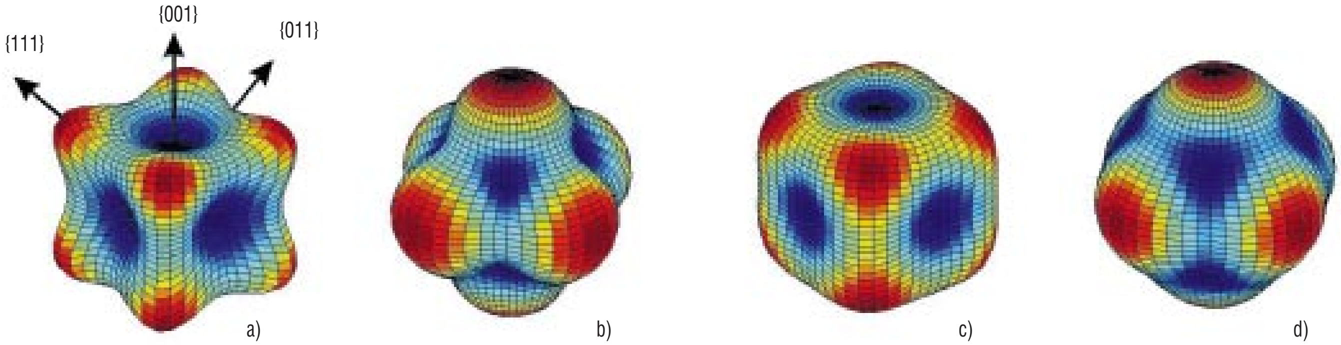

FIGURE 1. Dependence of Young's modulus E (a) and c)) and Poisson's ratio ν (b) and d)) on the direction *hkl* in the cubic crystal lattice for Ni. The case of the single crystal is represented by a) and b), whereas c) and d) show E(*hkl*) and n(*hkl*), respectively, as they would be obtained from a set of crystallites which have been selected out of an aggregate of randomly oriented grains. The selected crystallites have in common that for a certain *hkl* their lattice vectors are parallel.

Modern engineering analysis techniques, used to ensure that parts in e.g. bridges, airplanes, or automobiles will survive the stresses of use, rely on understanding the proportionality between stress and strain. For many applications the description of the proportionality between stress and strain in terms of isotropic, i.e. independent of direction, elastic constants is still sufficient, the knowledge of these constants for anisotropic cases becomes increasingly important for manufacturing processes, for micromechanical modeling of materials behavior, as well as for custom tailoring new composite materials. For materials which are crystalline on some length scale, anisotropy begins at the grain size level (single crystal elastic constants) and extends as far as anisotropy can be introduced into the material.

This macroscopic anisotropy is induced by two basic effects — a preferred orientation of the crystal lattice of the constituent grains and/or a preferred grain shape distribution. A preferred grain shape distribution means that grains or inclusions have a non-spherical shape on average and they are aligned to some common axis as well. This effect is not necessarily connected to the first one.

The anisotropy of elastic properties on a macroscopic scale (≈1 mm) can be readily measured by straining the specimen or by ultrasonic resonance. However, these methods fail in cases in which the microscopic scale is of interest. Examples are precipitations or inhomogeneities of other phases whose elastic constants are unknown but determine nonetheless the strength of the composite or alloy as a whole. The goal can therefore be formulated as the determination of the anisotropic or single crystal elastic constants on the microscopic scale. This can be achieved by diffraction which provides information about the strain and the elastic response of the crystal lattice for a particular direction [hkl].

These so called diffraction elastic constants (DEC) describe the elastic response of a particular family of lattice planes in a certain group of grains with the appropriate orientation to an applied load. Although the DEC are a feature of the polycrystal they can be readily compared to the directional dependence of the elastic constants in a single crystal (Fig. 1).

The smoothing effect for the 'aggregate' constant is a result of the fact that each of the grains in the polycrystal is surrounded by other, not necessarily randomly oriented grains. The elastic response of the selected grains is therefore somewhat obstructed in comparison to the single crystal. Thus, probing the DEC can provide a wealth of information about the average local conditions on the grain size level.

Since its commissioning the residual stress diffractometer at the thermal beamline BT8 has been used for a variety of engineering-applications-related measurements as well as for basic studies of the elastic behavior of materials. In the course of these experiments a method has been developed which allows the determination of single crystal elastic constants from measurements on polycrystals. This is done experimentally by loading a

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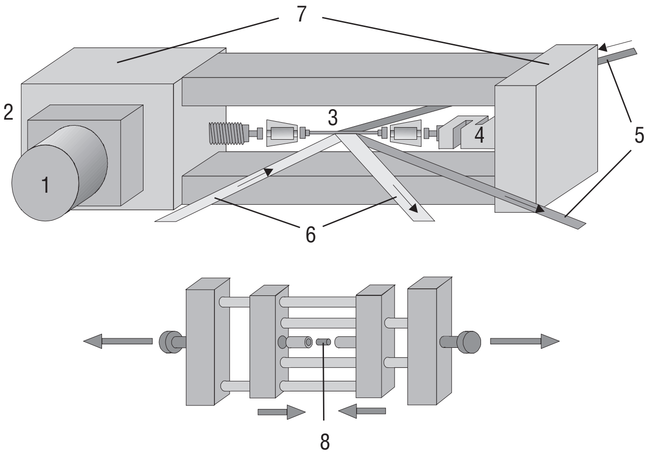

FIGURE 2. Schematic of the stress rig.

specimen in a stress rig and measuring the lattice response normal and parallel to the load direction (Fig.2 and Fig. 3).

1	stepping motor, resolution 1:360
2	gear, reduction 1:2500
3	tensile bar
4	10 kN load cell
5	beam in transmission (Young's modulus)
6	beam in reflection (Poisson's ratio)
7	stainless steel frame
8	compression sample in compression adapter

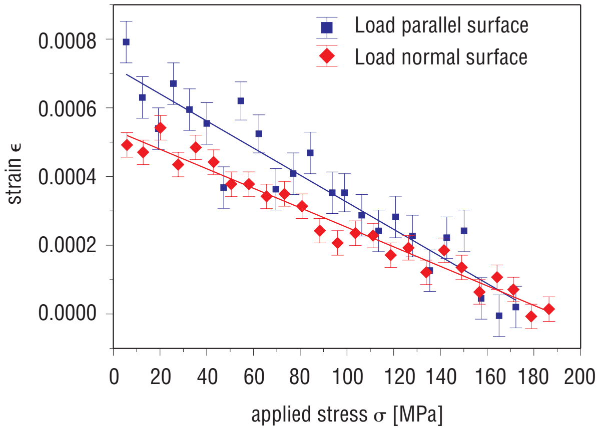

FIGURE 3. Lattice strain response in a transmission-compression setup for a γ-Al_20_3 plasma sprayed thermal barrier coating. Load experiments have been carried out normal and parallel to the coating surface. The difference in the slopes is due to the anisotropy of the sample

These experimental results can be compared to models which calculate the DEC from the single crystal constants [1]. These models can be reversed in a way which considers the single crystal elastic constants as unknown parameters [2,3]. This way the problem can be expressed as a least squares loop in which the single crystal elastic constants are refinable parameters.

Possible applications of the method are to materials which cannot or can only under great difficulties be synthesized as sufficiently large single crystals. Examples are γ' precipitations in γ/γ' hardened superalloys or metastable phases as plasma sprayed γ-Al_2O_3. γ' precipitates exist, strictly speaking, only within the equilibrium of the two phase compound, which therefore also requires the determination of their elastic constants from the composite. Thus, in these cases the method may provide the only available tool for determining their single crystal elastic constants.

REFERENCES

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