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Constitutive Description of Large Elastic Deformations in Diamond and Silicon Crystals from First-Principles M. SALVETTI, MIT, S. DUCHENNE, Mines ParisTech, D.M. PARKS, N. MARZARI, MIT — Within a continuum approach, the prediction of the mechanical response of single crystals at large elastic deformations relies on the accurate description of the strain energy density function Ψ. The coupling of hydrostatic and deviatoric terms at high compressions is of particular interest for applications, and the effect is generally not taken into account by current models available in the literature [1,2]. We present a general approach that leads to the construction of strain energy density functions of cubic single crystals based on data obtained from density functional theory (DFT) calculations. We connect the deformation-induced energy changes and Cauchy stress calculated from DFT calculations to the Lagrangian description frequently adopted within the continuum theory of hyperelasticity [3]. In particular, we adopt a coordinate–free invariant formulation [4] that intrinsically preserves the properties of the cubic symmetry group. We present results on diamond and silicon single crystals, and highlight both similarities and striking differences. [1] R.G.Veprek *et. al*, *Mater. Sci. Eng. A* **4248**, 366-378 (2007) [2] B.P Gearing, L. Anand, *Int. J. Solids Struct.* **41**, 827-845 (2004) [3] A.N. Norris, *J. Mech. Mater. Struct.* **3**, No.2, 243-260 (2008) [4] J.P. Boehler, *Z. Angew. Math. Mech.* **59**, 157-167 (1979)

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