Ackland Replies: In her Comment [1] Gupta refers to the calculated densities of states from a recent Letter [2] on delayed hydride cracking. She shows that the published densities of states are at variance with calculations using the LMTO-ASA method.

In [2] it was shown that stoichiometric ϵ-ZrH_2 exhibited a tetragonal distortion away from a hypothetical cubic fluorite structure for ZrH, and that these two were nonequivalent tetragonal distortions with $c > a$ and $c < a$ which give rise to a bistable crystal structure, the observed structure being dependent on the local stress field.

The densities of states shown in Fig. 3 of [2] are in error although the original calculations are not. The energy scale has been reversed and the band structures misinterpreted on that basis. Revised band structures with a corrected energy scale and calculated using a finer k-point mesh with linear interpolation are presented in Fig. 1, where qualitative agreement with the LMTO-ASA structures [1] is observed, in particular, the metallic nature of the material and the peak in the density of states at the Fermi energy of the cubic structure.

Since the hypothetical cubic ZrH_2 structure is not the δ-ZrH_{2-x} structure observed as precipitates in α-zirconium, and the embrittling mechanism is independent of the nature of the driving force behind this hypothetical phase transition, the other conclusions of the paper are unaffected.

As is well known, the convergence of energy differences with k-point sampling is far more rapid than that of the details of the band structure [3], and the key point regarding the bistability of the distortion is unaffected. It is unfortunate that the LMTO-ASA calculations have not attempted to address this central point: The mistake in the original band structure figure has no bearing on the delayed hydride cracking mechanism.

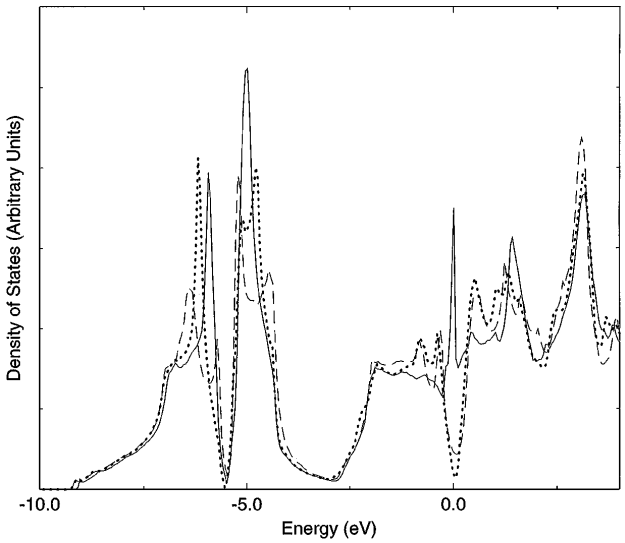

FIG. 1. Electronic density of states for cubic ZrH_2 (solid lines) and the two minimum energy tetragonal ZrH_2 (dots: $c < a$; dashes: $c > a$). A previous version of the figure was inadvertently printed backward in Ref. [2]. The zero of energy is taken at the Fermi energy.

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