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Stability of strained monohydride H:Si(105) and H:Ge(105) surfaces CRISTIAN V. CIOBANU, Colorado School of Mines, RYAN M. BRIGGS, Colorado School of Mines — We report atomic scale studies of the effect of applied strain and hydrogen environment on the reconstructions of the (105) Si and Ge surfaces. Surface energy calculations for monohydride-terminated (001) and (105) reconstructions reveal that the recently established single-height rebonded model is unstable not only with respect to (001), but also in comparison to other monohydride (105) structures. This finding persists for both Si and Ge, for applied biaxial strains from -4% to 4% , and for nearly the entire relevant domain of the chemical potential of hydrogen, thus providing a thermodynamics perspective on the recently observed H-induced destabilization of the Ge(105) surface.

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