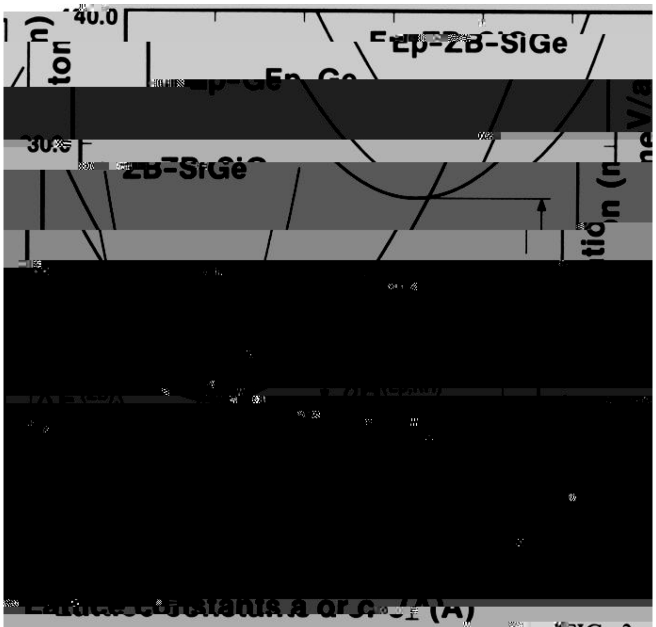

FIG. 3. Energy of bulk Ge, zinc-blende (ZB) SiGe, and rhombohedral (RH) SiGe as functions of the lattice constant a, and for epitaxially (Ep) confined (to $a_{Si}=5.387$ Å) ZB and RH SiGe as a function of c. For each curve the zero of the energy scale was adjusted such that the minimum of the curve gives the enthalpy of formation. ΔE_{ss} denotes the substrate strain; the shaded area denotes the *negative* enthalpy δH of Ep-RH SiGe. Energy cutoff of [illegible] Ry was used.