$\frac{1}{2}$ stat. (b) 223, 369 (2001)

 $\frac{1}{2}$ $\frac{1}{2}$

 \mathbf{m} structure to compound semiconductors are incorrect incorrect incorrect incorrect incorrect incorrect incorrect \mathbf{m}_c and so are incorrect \mathbf{m}_c many of the assigned NaCl structure α structure has been proposed theories of the CsCl structure has been proposed theories of the CsCl structure has been proposed theories of the CsCl structure has been proposed theor r_{α} , r_{α} 13, 15, 21, 22, $1/r_{\alpha}$, r_{α} As, M, \mathbf{M} As, M, M, \mathbf{M} but was set that \mathbf{M} and $\mathbf{y} = \mathbf{y} = \mathbf$

 \sim 3. Phonon dispersion dispersion dispersion dispersion of \mathbb{R} in the NaCle \mathbb{R} $\mathbf{s} = \mathbf{b}$ at the equilibrium volume $\mathbf{b} = \mathbf{b}$ ₁ $\mathbf{b} = \mathbf{1}$ $\frac{1}{\cdot}$ and at $\begin{array}{ccccccc} \bullet & \bullet & \bullet & \bullet & \bullet\end{array}$ $=\frac{-3}{1}$. Since \mathcal{A} in the Nacl structure is the NaCl structu $m_{\rm m}$, there is no LO/TO splitting at the $m_{\rm m}$ splitting at the $m_{\rm m}$ \mathbf{M}_{α} , \mathbf{M}_{α} , \mathbf{M}_{α} , \mathbf{M}_{α} , \mathbf{M}_{α} $m \rightarrow M$ are not $\mathbf{w}_i = 0$ for \mathbf{w}_i and \mathbf{w}_i and \mathbf{w}_i optimization with respect to the remaining \mathbf{v}_1 d degrees of d freedom (as d , \mathbf{M} , \mathbf{M} and \mathbf{M} and \mathbf{M} . 22 , 29), and Λ in \mathbf{M}_{α} in \mathbf{M}_{α} in \mathbf{M}_{α} in \mathbf{M}_{α} in \mathbf{M}_{α} increase it to a few tens of meV/atom. $T_{\rm{max}}$ the $T_{\rm{max}}$ the $T_{\rm{max}}$ structure cannot cannot cannot cannot cannot cannot cannot cannot cannot e_n in GaP at an ambient temperatures the set ambient temperature temperature temperature temperature temperatures that the set of t \P since it becomes \P by a \mathbb{R} by a \mathbb{R} becomes dynamically unstable be- $\mathbf{f} = \mathbf{f} \mathbf{f} + \mathbf{f$ $\mathbf{W}_1 = \mathbf{y}_1 \mathbf{y}_2 = \mathbf{y}_2 \mathbf{y}_3 = \mathbf{y}_3 \mathbf{y}_4$ lent compounds \mathbf{M}_S in \mathbf{A} instability all exhibits the TA(\mathbf{M}_A instability all exhibits at $\mathbf{A}(\mathbf{C})$ the equilibrium volume of the NaCl structure $\mathbf{W}_{\mathbf{A}}$ structure in com- \mathbf{P} , \mathbf{A} , \mathbf{M} , \mathbf{W} , \mathbf{W} and \mathbf{A} and \mathbf{A} of \mathbf{A} phase, since the NaCl $\mathbf{A}(\mathbf{X})$ in the Matrix sets in one on \mathbf{A} in \mathbf{A} is the \mathbf{A} $f_{\text{min}} = \text{max}$ in max is naturally explaint in max phonon installation in the \mathbf{r}_1 I sables in the b-Sn structure The G-Sn structure 10 $\begin{array}{|c|c|c|c|c|}\n\hline\n\text{R} & \text{TA(X) phonon in} \\
\hline\n\text{NaOf Structure} & \text{M}' & \text{M} \\
\hline\n\end{array}$ $\mathbf{w}_{\mathbf{v}} = \mathbf{w} \mathbf{w} + \beta \mathbf{w}_{\mathbf{v}} - \mathbf{w}_{\mathbf{v}}$ $\frac{1}{2}$ $\frac{30-32}{10}$ in connection with the theory with the theory of the theory of the theory with the theory of the theory of the three terms of the t WWW. MINITED WARD AND THE WARD TO A STATE structural transition to the simple \mathbf{y} of the simple heaven \mathbf{y} \mathcal{L} gonal phase in \mathcal{L} and \mathcal{L} and \mathcal{L} shows \mathcal{L} in \mathcal{L} . The shows \mathcal{L} \wedge \wedge along the tetragonal company $\mathcal{A}_{\text{max}} = \left[00\hat{\xi}\right]$ $\mathcal{A}_{\text{max}} = \mathbf{W}$ for compounds in the b-Sn structure. We consider the bounds in the bounds β \mathbf{w}_i , \mathbf{w}_i and \mathbf{w}_i and \mathbf{w}_i and \mathbf{w}_i . Logislations \mathbf{w}_i \mathbf{m} is constant as in the constant in \mathbf{v}_i $\mathbf{y} = \mathbf{W}_\text{c}$, we find \mathbf{W}_c , we find the find \mathbf{W}_c \sim 4. \wedge \blacksquare of \mathbb{I}_{\wedge} \wedge \wedge \blacksquare \blacksquare \blacksquare \blacksquare atomic displacements of the unstable phonon \mathbf{u} ψ in a) π and b) π structures between ψ and by π tures. Institution of the structural motion \mathbf{X} in these modes

and \mathbf{w}_{max} in the \mathbf{w}_{max} \bullet $[00\xi] \wedge$ \blacksquare , $\xi \approx 0.5$ \wedge \mathcal{C} rapidly softens with increasing ioni- $\mathbf{y} = \begin{pmatrix} \mathbf{y} & \mathbf{$ $e^{\frac{i\pi}{2}}$ all α llandi ba $e^{\frac{i\pi}{2}}$ kall $e^{\frac{i\pi}{2}}$ \blacksquare quencias for A , \wedge \wedge \blacksquare $V = 5$ shown \mathcal{N} is an order that the this analysis is an order to \mathcal{N} present even in metallic white time \mathbf{v}_{max} $\mathbf{w} = \mathbf{w} \cdot \mathbf{w}$ and $\mathbf{w} = \mathbf{w} \cdot \mathbf{w}$ $L = \bigoplus_{n=1}^{\infty} \bigcap_{n=1}^{\infty} \bigcup_{n=1}^{\infty} \bigcap_{n=1}^{\infty} \bigcap_{n=1}^{\infty} \bigcup_{n=1}^{\infty} \bigcap_{n=1}^{\infty} \bigcap_{n=1}^$ 33 , \mathbf{M}_{\wedge} , is $\wedge \mathbf{M}_{\wedge}$ \sim \sim \sim Ref. 1.34). T_{max} in an analogy with the set of the s $A() \rightarrow \blacksquare$ \sim characterize the LO230-MINUX-MINUX-THE LO β -MINU \sim characterize as an λ intrinsic to the b-SN structure. In contrast to the real space explanation given \mathbf{F}_A for the NaCl TA(X) anomaly, the b-Sn instability is explained by reciprocal space argu- \mathcal{L}^{max} is caused by the shape of the shape of the shape vectors λ is nested wave vectors. and $[000\sin \theta]$. The $[33.100\sin \theta]$ is unstable $[000\sin \theta]$ is unstable θ parameters, and should eventually stabilize with increasing pressure. To illustrate the $\mathbf{I} = \mathbf{I} \wedge \mathbf{I}$ of stable superstructures $\mathbf{I} \times \mathbf{B}$ via $\mathbf{I} \times \mathbf{M}$ instability, the inset of inset of $\mathbf{I} \times \mathbf{B}$ $F \circ A$ depicts the structural motion of $\mathbf{X} = \mathbf{X} \mathbf{X}$ in the structural mode at $\mathbf{X} = \mathbf{X} \mathbf{X}$ \mathcal{A} , we have the set of \mathcal{A} and \mathcal{A}

Table 2), while for M ⁵ , there are seven such sets (the seventh to thirteenth rows (1–7) $\stackrel{\wedge}{\bullet}$ $\stackrel{\wedge}{\bullet}$ $\stackrel{\wedge}{\bullet}$ 2). $\frac{1}{2}$ model and the B10 crystal structure: Figure 3 crystal structure that will structure that wi result from \mathbf{M} the \mathbf{M} members of the \mathbf{M} members of the unstable \mathbf{M} members of the \mathbf{M} structure has P4/nmm symmetry. This is the term of $4, M$ -type 38 structure (B10) derived by a soft Maria \mathbf{M} and \mathbf{M} and \mathbf{M} atoms \mathbf{M} atoms are in \mathbf{M} α and α , \mathbb{L} . \blacksquare (100) α is \blacksquare , where α is a dimensionless in \blacksquare celling $\alpha \wedge \beta$ structure bar in the unit α structure B structure B structure α $\mathbf{h}_\mathbf{a} = \mathbf{w}_\mathbf{a}$, and $\mathbf{w}_\mathbf{a}$ is the shaded (001) $\mathbf{h}_\mathbf{a} = \mathbf{w}_\mathbf{a}$, and $\mathbf{w}_\mathbf{a} = \mathbf{w}_\mathbf{a}$ $s_{\rm sc}$ (Fig. 7c) the animal theory $\alpha_{\rm sc}$ arrows) so that $\alpha_{\rm sc}$ arrows $\alpha_{\rm sc}$ $\begin{equation} \mathcal{L}_{\mathcal{A}} \subset \mathcal{A} \subset$ $f: \mathbb{R}^n$ and \mathbb{R}^n and $f:=(001)$ and \mathbb{R}^n and $f:=(\mathbb{R}^n, \mathbb{R}^n)$ and \mathbb{R}^n $\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$ **W**₁ $\mathbf{M} = \begin{bmatrix} 2 \\ 1 \end{bmatrix} = [(\mathbf{0}/(1-\mathbf{1}))^2 + \frac{1}{4}]^{1/2}$

sidered as a distorted diatomic hepatomic hepatomic transformation 2 structure transforms into this structure transforms into the B2 structure transforms into the B2 structure transforms into the B2 structure transforms ture when (i) the hexagonal B2 faces (the (110) p. \mathbf{M}_n faces \mathbf{M}_n at the bottom of both of bottom $F(S) = \frac{1}{2} \int_{0}^{\infty} \frac{1}{\sqrt{N}} \exp\left(-\frac{N\sqrt{N}}{N}\right) \exp\left(-\frac{N\sqrt{N}}{N}\right) \exp\left(-\frac{N\sqrt{N}}{N}\right) \exp\left(-\frac{N\sqrt{N}}{N}\right)$ $\frac{1}{2}$ atoms in a property in alternative contraction as $\frac{1}{2}$ (110) $\frac{1}{2}$ and $\frac{1}{2}$ and $\frac{1}{2}$ and $\frac{1}{2}$ $\mathbf{X} \cdot \mathbf{A}$ and $\mathbf{A} \cdot \mathbf{A}$ is $\mathbf{A} \cdot \mathbf{A}$ in $\mathbf{A} \cdot \mathbf{A}$ in $\mathbf{A} \cdot \mathbf{A}$ in $\mathbf{A} \cdot \mathbf{A}$ is $\mathbf{A} \cdot \mathbf{A}$ in $\mathbf{A} \cdot \mathbf{A}$ is $\mathbf{A} \cdot \mathbf{A}$ in $\mathbf{A} \cdot \mathbf{A}$ is $\mathbf{A} \cdot \mathbf{A}$ is \blacksquare Heving its symmetry and B10 an candidate structures that can replace that can replace the B2 structure $(2-\omega)(\sim .7$ c and 8), we now compute the static total energies of \mathbf{r}_min in the cell-internal and cell-inte external structural parameters allowed by symmetry. We find that λ B_{λ} phases are lower in energy than the B2 phase at the volumes λ is the B2 is the B expected to be stable according to \mathbb{R}^n and \mathbb{R}^n and the transmissions alone the transmission \mathbb{R}^n \mathbb{S} into the B₁ p_{hase}, \mathbb{S} ₁₀ is the lowest energy phase. At \mathbb{S} ₁₀ = 0.50, the λ \mathbb{R} of 1 is 10 phase is λ \mathbb{R} phase 1 and 2 phase 29 meV λ lower by \mathbf{A} as the pressure is raised function function function \mathbf{M}_i of \mathbf{M}_i s_{max} . At $\neq 0$: $= 0.42$, the total energy differences are 73 meV between $\frac{10}{10}$ and $\frac{10}{10}$ $2^{\frac{1}{2}}$, -92λ , -92λ , 2.