Electronic Supplementary Materials

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The mechanical, acoustical, and optical properties of several Li-Si alloys: a first-principles study

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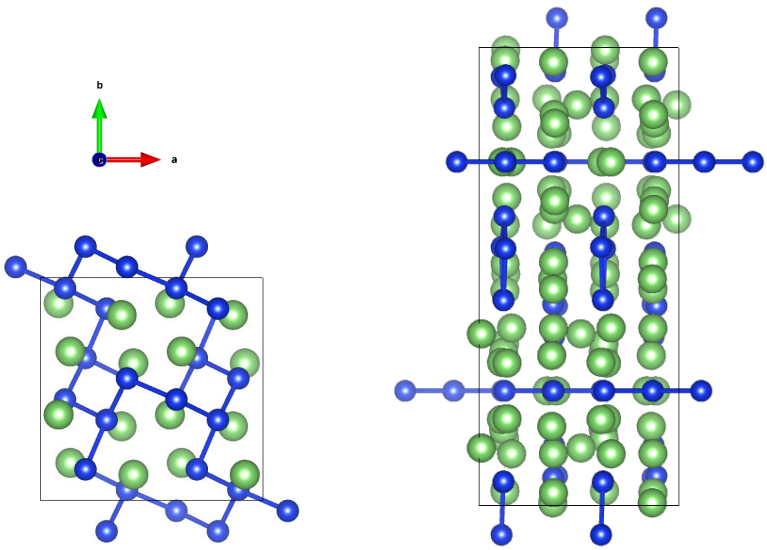
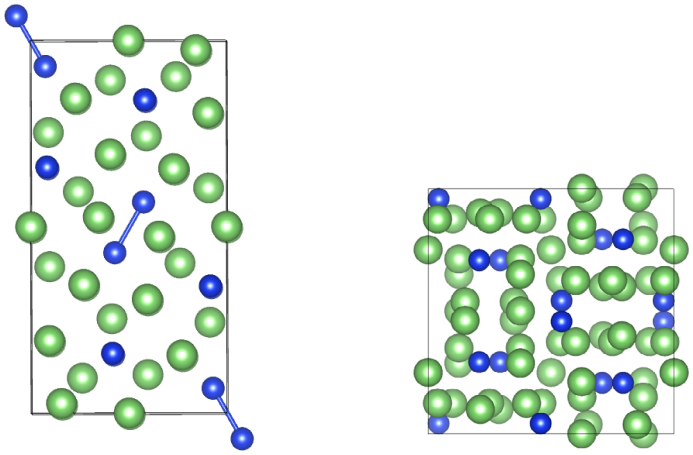
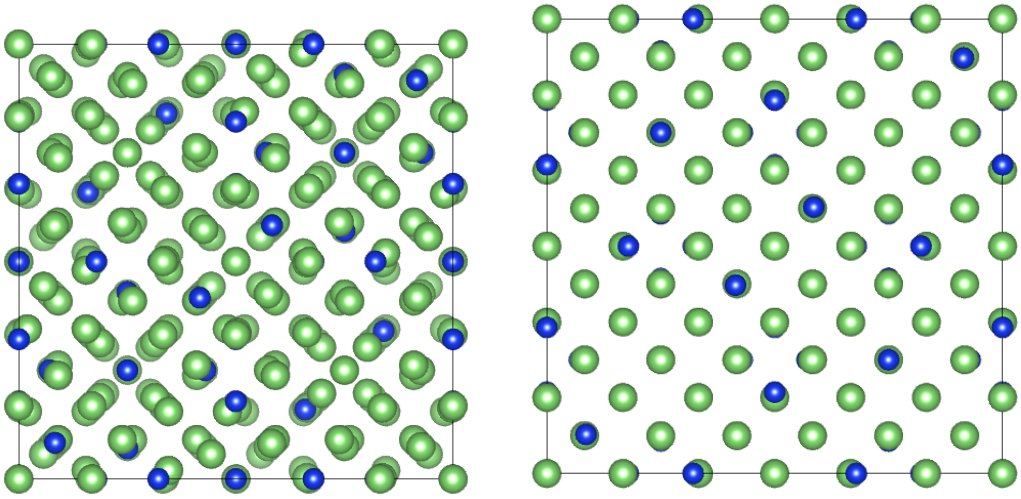


LiSi $Li_{12}Si_7$



$Li_{13}Si_4$ $Li_{15}Si_4$



$Li_{17}Si_4$ $Li_{22}Si_5$

Fig. S1 Crystal structures of the Li-Si alloys (● denotes Li atom, ● denotes Si atom)

Data S1 Equations

For tetragonal structure, B_V and G_V in the Voigt approximation are given as:

$$\begin{aligned} B_V &= \frac{2(C_{11}+C_{12})+C_{33}+4C_{13}}{9} \\ G_V &= \frac{M+3C_{11}-3C_{12}+12C_{44}+6C_{66}}{30} \end{aligned} \tag{S1}$$

Reuss shear modulus B_R and G_R are given as:

$$\begin{aligned} B_R &= \frac{C^2}{M} \\ G_R &= \frac{15}{\frac{18B_V}{C^2}+\frac{6}{C_{11}-C_{12}}+\frac{6}{C_{44}}+\frac{3}{C_{66}}} \end{aligned} \tag{S2}$$

where $\begin{aligned} M &= C_{11}+C_{12}+2C_{33}-4C_{13} \\ C^2 &= (C_{11}+C_{12})C_{33}-2C_{13}^2 \end{aligned}$.

For cubic structure, the Voigt and Reuss elastic moduli are given as [41, 42]:

$$\begin{aligned} B_V &= B_G = \frac{C_{11}+2C_{12}}{3} \\ G_V &= \frac{C_{11}-C_{12}+3C_{44}}{5} \\ G_R &= \frac{5C_{44}(C_{11}-C_{12})}{4C_{44}+3(C_{11}-C_{12})} \end{aligned} \tag{S3}$$

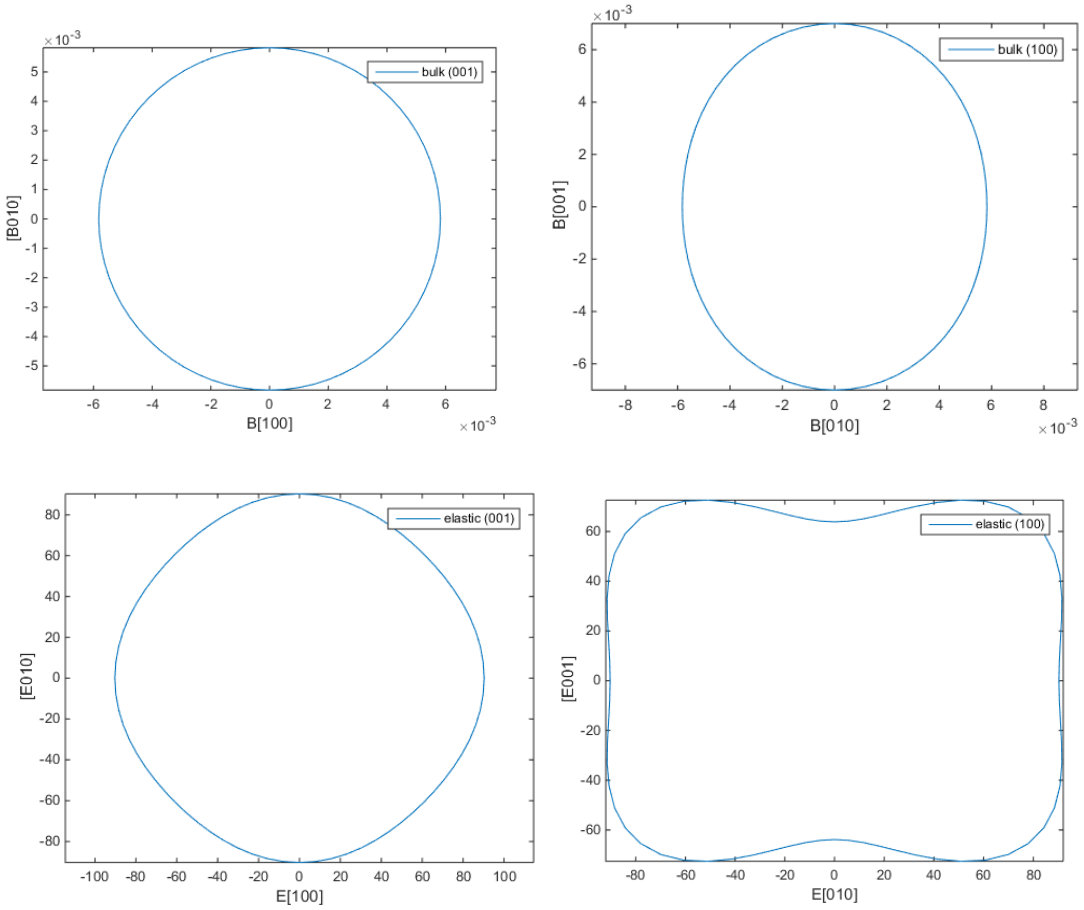
For orthorhombic structure, the Voigt and Reuss elastic moduli can be obtained by the following equations [40]:

$$\begin{aligned} B_V &= \frac{C_{11}+C_{22}+C_{33}+2C_{12}+2C_{13}+2C_{23}}{9} \\ G_V &= \frac{C_{11}+C_{22}+C_{33}-C_{12}-C_{13}-C_{23}}{15}+\frac{C_{44}+C_{55}+C_{66}}{5} \end{aligned} \tag{S4}$$

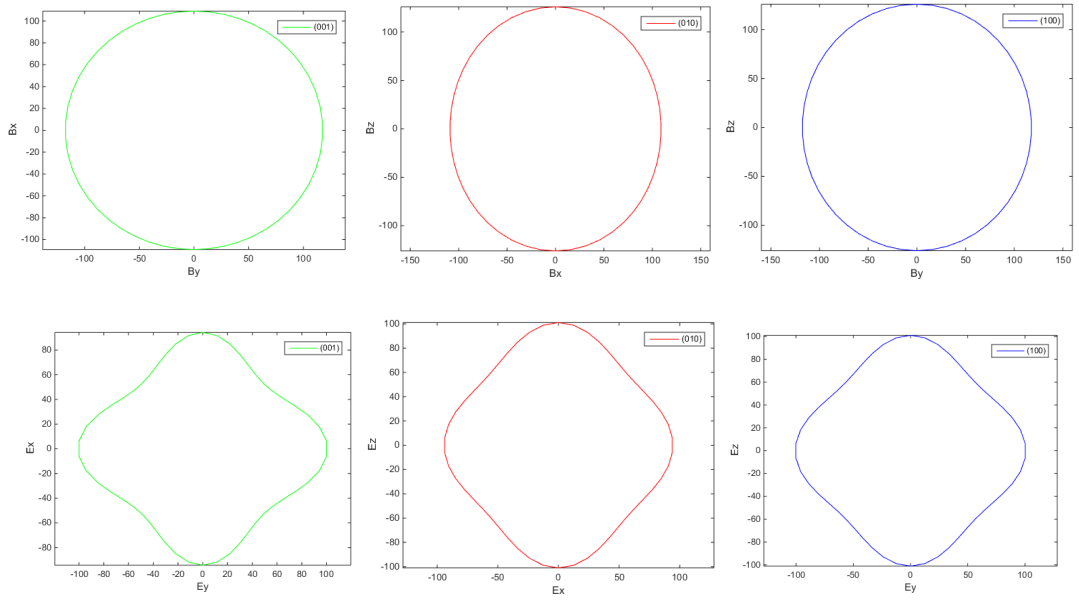
$$\begin{aligned} B_R &= \frac{1}{s_{11}+s_{22}+s_{33}+2(s_{12}+s_{13}+s_{23})} \\ G_R &= \frac{15}{4(s_{11}+s_{22}+s_{33})-4(s_{12}+s_{13}+s_{23})+3(s_{44}+s_{55}+s_{66})} \end{aligned} \tag{S5}$$

where s_{ij} are the elastic compliance constants of $Li_{12}Si_7$ and $Li_{13}Si_4$.

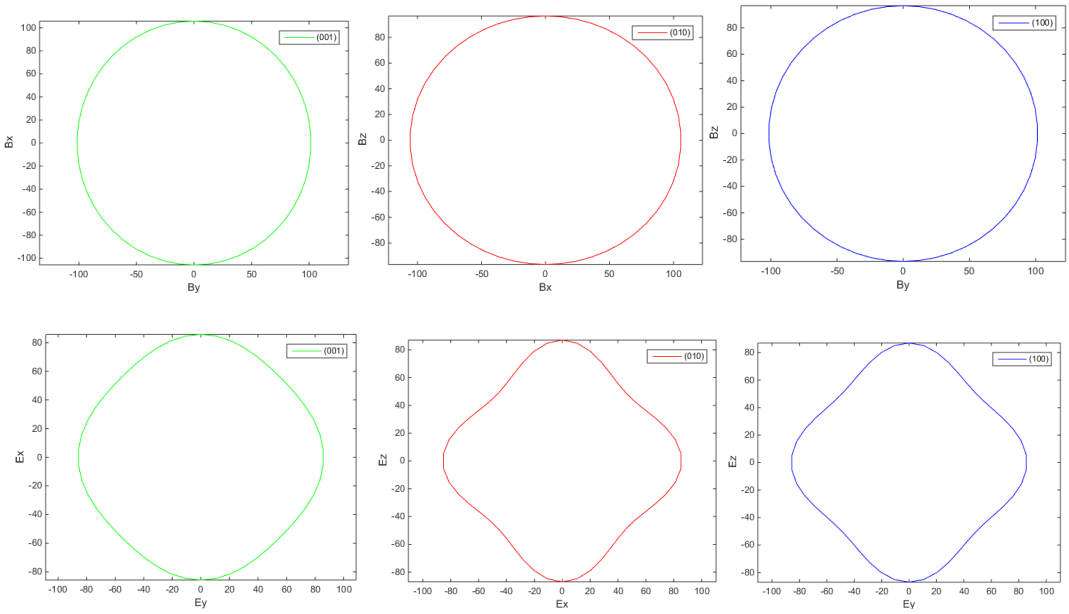
LiSi



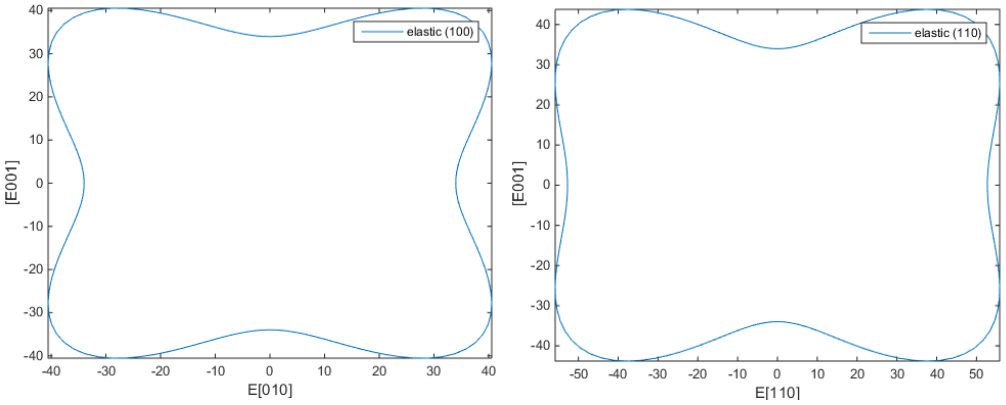
$Li_{12}Si_7$



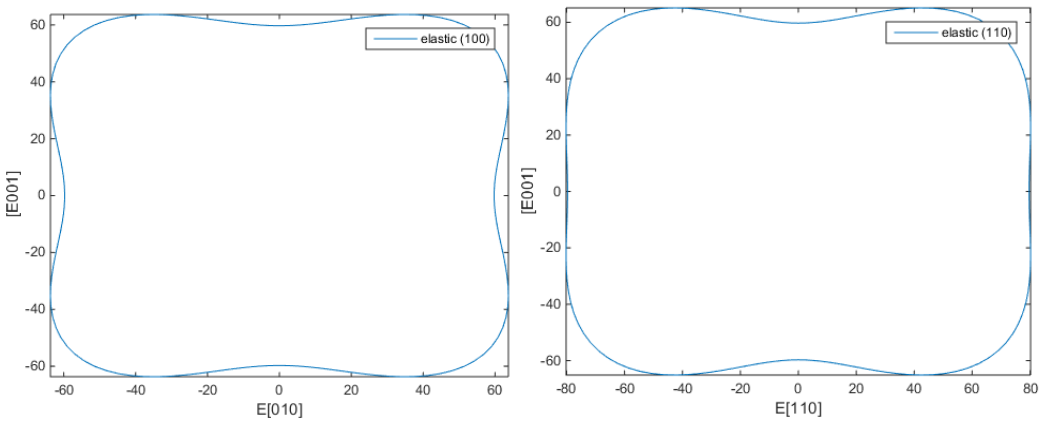
$Li_{13}Si_7$



$Li_{15}Si_4$



$Li_{17}Si_4$



$Li_{22}Si_5$

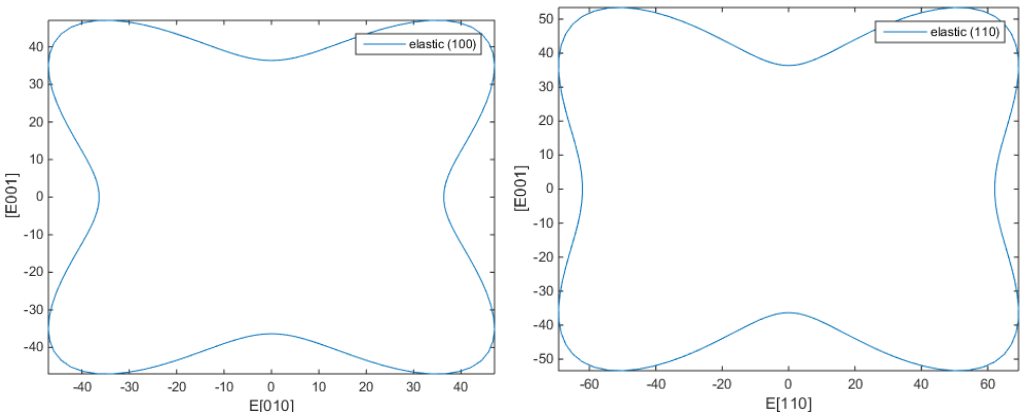


Fig. S2 Directional bulk modulus and Young's modulus of the studied materials on other atomic planes

Table S1 Elastic compliance constants of the studied Li-Si alloys

Alloy	s_{11}	s_{12}	s_{13}	s_{22}	s_{23}	s_{33}	s_{44}	s_{55}	s_{66}
LiSi	0.0110739	−0.0009226	−0.0043291	–	–	0.0156591	0.0224038	0.0262336	–
$Li_{12}Si_7$	0.0106047	0.0004549	−0.0009803	0.0099275	−0.0009743	0.0098927	0.0307229	0.0305430	0.0357988
$Li_{13}Si_4$	0.0116619	−0.0014284	−0.0007859	0.0116314	−0.0003616	0.0114886	0.0347302	0.0382378	0.0303513
$Li_{15}Si_4$	0.0263472	−0.0079098	–	–	–	–	0.0304052	–	–
$Li_{17}Si_4$	0.0167435	−0.0034329	–	–	–	–	0.0235940	–	–
$Li_{22}Si_5$	0.0275127	−0.0084514	–	–	–	–	0.0263036	–	–