Supplementary Information

A first-principles study of the structural, mechanical, and electronic properties of precipitates of Al_2Cu in Al-Cu alloys

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1 The generalized Hook's law

A proportional elastic constant C_{ij} can be expressed as

$$\sigma_i = \sum_{j=1}^{6} C_{ij}\varepsilon_j \qquad (S1)$$

where σ is stress and ε is strain

2 the mechanical stability criteria for crystals

For a cubic structure, the mechanical stability criteria are [Long2013]

$$\begin{cases} C_{11} > 0; C_{44} > 0 \\ C_{11} - C_{12} > 0 \\ C_{11} + 2C_{12} > 0 \end{cases} \tag{S2}$$

For a tetragonal structure [Shein2011],

$$\begin{cases} C_{ii} > 0, i = 1,2,3,4,5,6 \\ C_{11} - C_{12} > 0 \\ C_{11} + C_{33} - 2C_{13} > 0 \\ 2C_{11} + C_{33} + 2C_{12} + 4C_{12} > 0 \end{cases} \tag{S3}$$

For an orthorhombic crystal [Zhou2009],

$$\begin{cases} C_{ii} > 0, i = 1,2,3,4,5,6 \\ C_{11} + C_{22} - 2C_{12} > 0 \\ C_{11} + C_{33} - 2C_{13} > 0 \\ C_{22} + C_{33} - 2C_{23} > 0 \\ C_{11} + C_{22} + C_{22} + 2(C_{12} + C_{13} + C_{23}) > 0 \end{cases} \tag{S4}$$

and for a monoclinic structure, the more complicated criteria are expected [Watt1980]

$$\begin{cases} C_{ii} > 0, i = 1,2,3,4,5,6 \\ C_{22}C_{33} - C_{23}^2 > 0; C_{33}C_{55} - C_{35}^2 > 0; C_{44}C_{66} - C_{46}^2 > 0 \\ C_{11} + C_{22}C_{33} + 2(C_{12} + C_{13} + C_{23}) > 0 \\ C_{22}\left(C_{33}C_{55} - C_{35}^2\right) + 2\left(C_{23}C_{25}C_{35} - C_{25}^2\left(C_{55} - C_{33}\right)\right) > 0 \\ 2\begin{bmatrix} C_{15}C_{25}\left(C_{33}C_{12} - C_{13}C_{23}\right) + C_{15}C_{35}\left(C_{22}C_{13} - C_{12}C_{23}\right) \\ + C_{25}C_{35}\left(C_{11}C_{23} - C_{12}C_{13}\right) - C_{15}^2\left(C_{22}C_{33} - C_{23}^2\right) \\ + C_{25}^2\left(C_{11}C_{33} - C_{13}^2\right) + C_{35}^2\left(C_{11}C_{22} - C_{12}^2\right) \end{bmatrix} \\ + C_{55}\left(C_{11}C_{22}C_{33} - C_{11}C_{23}^2 - C_{22}C_{13}^2 - C_{33}C_{12}^2 + 2C_{12}C_{13}C_{23}\right) > 0 \end{cases} \tag{S5}$$

4 The bulk modulus and shear modulus

The bulk modulus and shear modulus of materials with Voigt-Reuss-Hill approximation [Hill1952] can be expressed as

$$\begin{cases} B = \left(\dfrac{B_V + B_R}{2}\right) \\ G = \left(\dfrac{G_V + G_R}{2}\right) \end{cases} \tag{S6}$$

where B_V, B_R, G_V and G_R are Voigt bulk modulus, Reuss bulk modulus, Voigt shear modulus and Reuss shear modulus, respectively, which can be calculated from the elastic constants as follows,

$$\begin{cases} B_V = \frac{1}{9}(C_{11} + C_{22} + C_{33}) + \frac{2}{9}(C_{12} + C_{13} + C_{23}) \\ B_R = [S_{11} + S_{22} + S_{33} + 2(S_{12} + S_{13} + S_{23})]^{-1} \\ G_V = \frac{1}{15}(C_{11} + C_{22} + C_{33} - C_{12} - C_{13} - C_{23}) + \frac{1}{5}(C_{44} + C_{55} + C_{66}) \\ G_R = 15[4(S_{11} + S_{22} + S_{33}) - 4(S_{12} + S_{13} + S_{23}) + 3(S_{44} + S_{55} + S_{66})]^{-1} \end{cases} \tag{S7}$$

where S_{ij} is the elastic compliance constants and can be obtained from elastic constants.

5 Young's modulus and Poisson's ratio

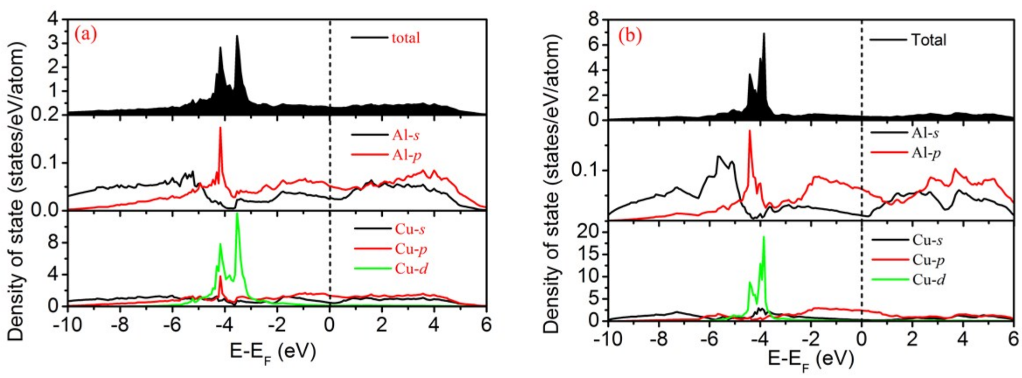
The Young’s modulus of a crystal can be obtained using following equation

$$E = \frac{9GB}{3B + G} \tag{S8}$$

and the Poisson’s ratio is given by

$$\nu = \frac{E}{2G} - 1 \tag{S9}$$

6 The electronic density of state for the Al-Cu precipitates



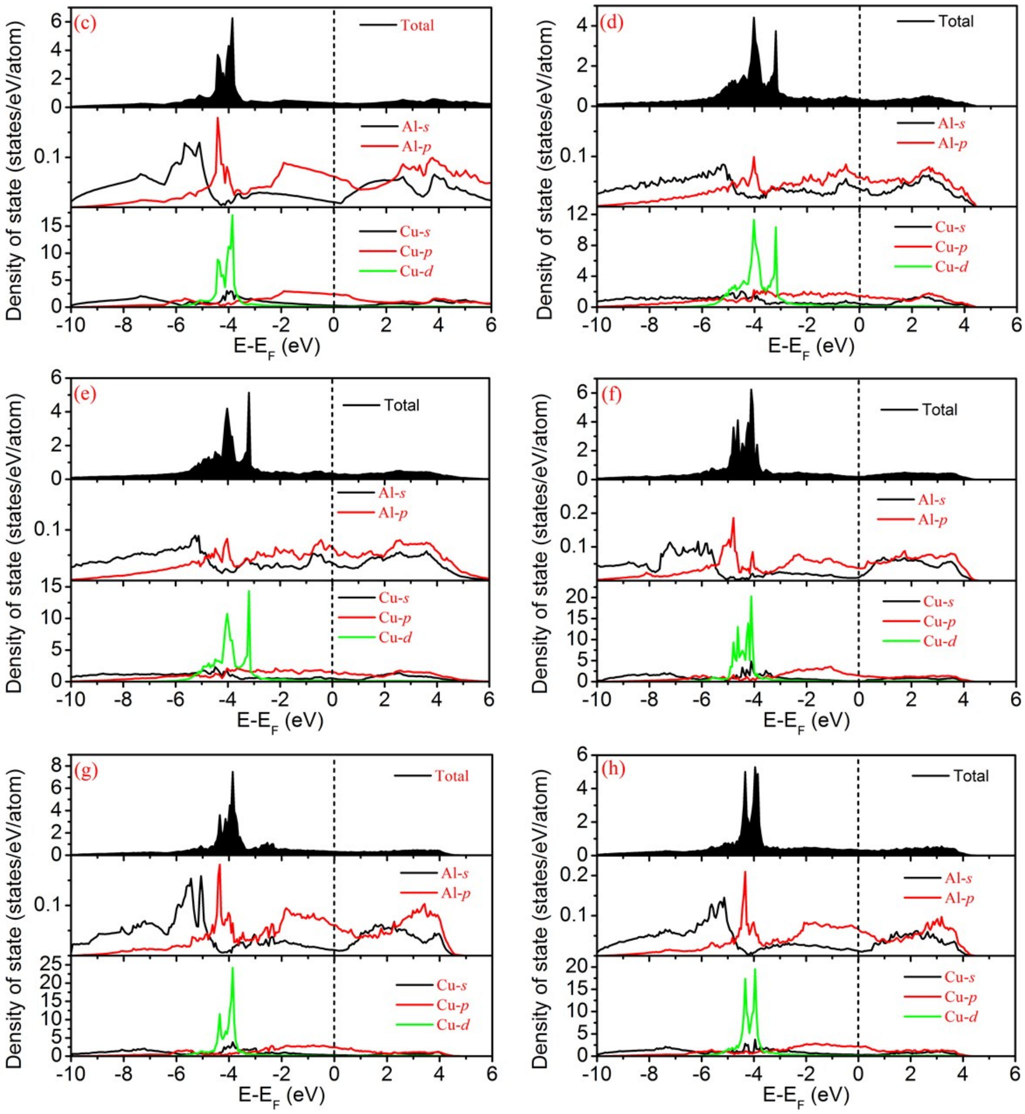


Fig. S1 Calculated total and partial electronic densities of state for the precipitates. (a): θ''-Al_3Cu, (b): θ'-Al_2Cu, (c): θ'_C-Al_2Cu, (d): θ'_O-Al_2Cu, (e): θ-Al_2Cu, (f): θ'_D-Al_5Cu_3, (g): θ'_t-$Al_{11}Cu_7$, (h): θ''_t-$Al_{13}Cu_5$ (the density of states for Cu-*s* and Cu-*p* were enlarged by 20 times). The Fermi energy level is set to Zero and marked by a vertical line.

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