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ABSTRACT

In order to clarify the physical meaning of the eigenvector of the atomic elastic stiffness matrix, $B_{ij} = \Delta \sigma_{ij}/\Delta \varepsilon_{ij}$, static calculations of uniaxial tension are performed on various fcc, bcc, and hcp metals with four different embedded atom method (EAM) potentials. Many fcc metals show instability for the constant volume mode, or the eigenvector of $(\Delta \varepsilon_{xx}, \Delta \varepsilon_{yy}, \Delta \varepsilon_{zz}) = (\pm 1, \pm 1, 0)$, under the [001] tension. Bcc also loses resistance against other constant volume mode, $(\Delta \varepsilon_{xx}, \Delta \varepsilon_{yy}, \Delta \varepsilon_{zz}) = (\pm 1, \pm 1, \pm 2)$, in the [001] tension. Hcp shows shear modes $\Delta \gamma_{yz}$ and $\Delta \gamma_{zx}$ under the [0001] tension, which correspond to atom migration by dislocation on the slip plane. Similar shear modes appear in the [111] tension of fcc and [110] tension of bcc. Hcp also changes the mode to constant volume and shear in the [010] tension, which imply the deformation in the pyramidal and prismatic planes.

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I. INTRODUCTION

We have proposed a deformation mode analysis based on a 6 × 6 matrix of atomic elastic stiffness (AES), $B_{ij} = \Delta \sigma_{ij}/\Delta \varepsilon_{ij}$, for each atom to discuss local deformation such as crack propagation and dislocation glide. $\Delta \sigma_{ij}$ is the change in the atomic stress, $\Delta \varepsilon_{ij}$ is that in the strain, and the subscripts $i, j$ are the Voigt notation of $i, j = 1 \sim 6 = xx, yy, zz, yz, zx, xy$. We can construct the eigenequation of $B_{ij} \Delta \varepsilon_i = \eta_{ij} \Delta \varepsilon_i$ for each atom and obtain six eigenvalues $\eta^{(1)} \sim \eta^{(6)}$. This process is equivalent to the diagonalization of the matrix $B_{ij}$, and the six eigenvalues are the diagonal elements aligned in ascending order. If atoms have negative eigenvalues, they can be regarded as “unstable” from the relation of $\Delta \sigma_{ij} = B_{ij} \Delta \varepsilon_j = \eta_{ij} \Delta \varepsilon_i$. The corresponding eigenvector $(\Delta \varepsilon_i) = (\Delta \varepsilon_1, \ldots, \Delta \varepsilon_6)^T = (\Delta \varepsilon_{xx}, \ldots, \Delta \varepsilon_{yz})^T$ for $\eta^{(4)} < 0$ atoms is also expected to reflect the deformation path. Here, superscript T means transpose to denote that the column vector is shown in the row vector form. In fact, the crack opening mode and the glide direction of the dislocation core were visualized by the principal axes of the strain tensor $(\Delta \varepsilon_{ij})$ (where $i, j$ are the Cartesian indices of $x, y, z$) of which components are those of the eigenvector $(\Delta \varepsilon_i)$ of the $\eta^{(4)} < 0$ atoms.

Nishimura et al. also evaluated $B_{ij}$ in the buckling simulation of a multi-wall carbon nanotube (MWCNT) and reported that the global buckling of MWCNT is triggered by the emergence of $\lambda^{(3)}_{22} < 0$ atoms ($\lambda^{(3)}_{22}$ corresponds to $\eta^{(12)}$), after all the atoms become $\lambda^{(1)}_{11} < 0$ in MWCNT. They also revealed that the corresponding eigenvectors are $(0, 0, 0, 0, 0, \gamma_{22}, 0)^T$ for $\lambda^{(1)}_{11} < 0$ (in-plane shear in each CNT surface) and $(0, 0, 0, 0, 0, \gamma_{12}, 0)^T$ for $\lambda^{(22)}_{22} < 0$ (out-of-plane shear) in the $(r, \theta, z)$ cylindrical coordinate. Thus, the eigenvector definitely suggests deformation mode; however, the diagonalization is performed in the six-dimensional space of $xx, yy, zz, yz, zx, xy$ so that the eigenvalue may have dependency on the coordinate, in contrast to the coordinate independence of the principal strain/stress of the tensor.

In the present study, the characteristics of the eigenvalue and eigenvector of $B_{ij}$ are discussed in static uniaxial tension for two different crystal orientation, in order to show the fundamental aspects of these quantities. Eight fcc, four bcc, and four hcp elements were calculated with embedded atom method (EAM) potential by Zhou et al. and compared with different EAM potential for Ni and Al by Voter et al., Fe by Finnis–Sinclair, and Mg by Liu et al.
II. EIGENVALUE AND EIGENVECTOR IN PERFECT LATTICE

As already indicated in our previous papers,1–4 the mathematical form of the atomic stress, $\sigma_i$, and the atomic elastic coefficients, $C_{ij}$, are easily formulated in the EAM potential; thus, both are directly calculated only with the atom configuration at each impact. $B_0^i$ can be evaluated with $C_{ij}$ and the stress contribution, e.g., $B^3_{11} = C_{11} + \sigma_1$, $B^3_{12} = C_{12} - (\sigma_1 + \sigma_2)/2$, and $B^3_{44} = C_{44} + (\sigma_1^2 + \sigma_2^2 + \sigma_3^2 - \sigma_1^2)/2$. In the no-load perfect lattice, $B_0^i$ coincides with $C_{ij}$ or the elastic coefficient of the crystal since all the atoms are same. Supposing isotropic elasticity, the $C_{ij}$ matrix is expressed as follows:

$$[C_{ij}] = \begin{bmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{bmatrix}$$

Table I. Elastic coefficients of fcc metals (unit: GPa).

| Elements  | Zhou  | Voter |
|-----------|-------|-------|
| Cu        | 169.6 | 124.0 |
| Ag        | 246.2 | 243.8 |
| Au        | 187.8 | 150.0 |
| Ni        | 140.7 | 140.0 |
| Cu$_{11}$ | 122.1 | 93.6  |
| Cu$_{12}$ | 75.7  | 45.9  |
| Cu$_{44}$ | 47.5  | 30.4  |
| Cu$_{11} - Cu_{12}$ | 234.5 | 343.2 |
| Pd        | 50.3  | 106.9 |
| Pt        | 88.6  | 100.6 |
| Pb        | 42.7  | 60.5  |
| Al        | 24.7  | 60.5  |
| Al$_{11}$ | 71.5  | 79.2  |
| Al$_{12}$ | 58.5  | 88.9  |
| Al$_{11} - Al_{12}$ | 234.5 | 343.2 |
| Al$_{2}$  | 50.3  | 106.9 |
| Al$_{3}$  | 42.7  | 60.5  |
| Al$_{4}$  | 24.7  | 60.5  |
| Al$_{11} - Al_{12}$ | 71.5  | 79.2  |
| Al$_{12}$ | 58.5  | 88.9  |
| Al$_{11} - Al_{12}$ | 234.5 | 343.2 |
| Al$_{2}$  | 50.3  | 106.9 |
| Al$_{3}$  | 42.7  | 60.5  |
| Al$_{4}$  | 24.7  | 60.5  |

Table II. Eigenvectors of $C_{ij}$ of fcc metals in the $x$[100], $y$[010], and $z$[001] coordinate systems with a strain perturbation of $\varepsilon_{22} = 0.001$. The solution for the shear components $\Delta \varepsilon_{yz}$, $\Delta \varepsilon_{xz}$ is equivalent to $(\Delta \varepsilon_{yz}, \Delta \varepsilon_{xz}) = (1, 0)$, $(0, 1)$.

| Elements   | Zhou  | Voter |
|------------|-------|-------|
| Cu        | ±0.71 | ±0.71 |
| Cu$_{11} - Cu_{12}$ | ±0.41 | ±0.41 |
| Cu$_{44}$ | 0.12  | 0.99  |
| Cu$_{11} - Cu_{12}$ | 0.99  | 0.12  |
| Cu$_{44}$ | 0.58  | ±0.58 |
| Cu$_{11} - Cu_{12}$ | 0.58  | ±0.58 |
| Cu$_{44}$ | 0.58  | ±0.58 |
| Cu$_{11} - Cu_{12}$ | 0.58  | ±0.58 |
| Cu$_{44}$ | 0.58  | ±0.58 |

Table III. Elastic coefficients of bcc metals (unit: GPa).

| Elements  | Zhou  | FS  |
|-----------|-------|-----|
| Fe        | 229.6 | 456.8 |
| Mo        | 135.5 | 166.7 |
| Ta        | 116.7 | 113.2 |
| W         | 94.1  | 290.1 |
| Fe$_{11}$ | 210.7 | 278.2 |
| Mo$_{11}$ | 201.9 | 199.2 |
| Ta$_{44}$ | 225.7 | 224.4 |
| W$_{44}$  | 301.5 | 300.9 |
| Fe$_{11} - Fe_{12}$ | 210.7 | 278.2 |
| Mo$_{11} - Mo_{12}$ | 201.9 | 199.2 |
| Ta$_{44} - Ta_{44}$ | 225.7 | 224.4 |
| W$_{44} - W_{44}$  | 301.5 | 300.9 |

Table IV. Eigenvectors of $C_{ij}$ of bcc metals in the $x$[100], $y$[010], and $z$[001] coordinate systems with a strain perturbation of $\varepsilon_{22} = 0.001$. The solution for the shear components $\Delta \varepsilon_{yz}$, $\Delta \varepsilon_{xz}$ is equivalent to $(\Delta \varepsilon_{yz}, \Delta \varepsilon_{xz}) = (1, 0)$, $(0, 1)$.

| Elements   | Zhou  | FS  |
|------------|-------|-----|
| Fe        | ±0.71 | ±0.71 |
| Mo        | ±0.41 | ±0.41 |
| Ta        | ±0.82 | ±0.82 |
| W         | 0.12  | 0.99  |
| Fe$_{11}$ | 0.58  | ±0.58 |
| Mo$_{11}$ | 0.58  | ±0.58 |
| Ta$_{44}$ | 0.58  | ±0.58 |
| W$_{44}$  | 0.58  | ±0.58 |

The characteristic equation of the $3 \times 3$ submatrix of the upper left is

$$det \begin{bmatrix} C_{11} - \eta & C_{12} & C_{12} \\ C_{12} & C_{11} - \eta & C_{12} \\ C_{12} & C_{12} & C_{11} - \eta \end{bmatrix} = 0$$

$$\Rightarrow (\eta - (C_{11} - C_{12}))^2 (\eta - (C_{11} + 2C_{12})) = 0$$

Table V. Elastic coefficients of hcp metals (unit: GPa).

| Elements  | Zhou  | Liu |
|-----------|-------|-----|
| Mg        | 60.2  | 60.2 |
| Co        | 24.2  | 24.2 |
| Ti        | 13.9  | 13.9 |
| Zr        | 20.2  | 20.2 |
| Mg$_{33}$ | 69.5  | 69.5 |
| Mg$_{66}$ | 18.0  | 18.0 |
| Mg$_{11} - Mg_{12}$ | 36.0  | 36.0 |

| Elements   | Zhou  | Liu |
|------------|-------|-----|
| Mg        | 284.9 | 284.9 |
| Co        | 162.2 | 162.2 |
| Ti        | 158.7 | 158.7 |
| Zr        | 63.4  | 63.4  |
| Mg$_{33}$ | 75.1  | 75.1  |
| Mg$_{66}$ | 67.7  | 67.7  |
| Mg$_{11} - Mg_{12}$ | 87.1  | 87.1  |

| Elements   | Zhou  | Liu |
|------------|-------|-----|
| Mg        | 24.2  | 24.2 |
| Co        | 13.9  | 13.9 |
| Ti        | 20.2  | 20.2 |
| Zr        | 69.5  | 69.5 |
| Mg$_{33}$ | 18.0  | 18.0 |
| Mg$_{66}$ | 36.0  | 36.0 |
| Mg$_{11} - Mg_{12}$ | 151.4 | 151.4 |
| \( n \) | \( \Delta \varepsilon_{xx} \) | \( \Delta \varepsilon_{xy} \) | \( \Delta \varepsilon_{xz} \) | \( \Delta \gamma_{yz} \) | \( \Delta \gamma_{zx} \) |
|-----|-----|-----|-----|-----|-----|
| 1   | 13.9 | 0   | 0   | 0   | 1   |
| 2   | 13.9 | 0   | 0   | 0   | 0   |
| 3   | 18.0 | 0   | 0   | 0   | 0   |
| 4   | 36.0 | ±0.71 | ±0.71 | 0 | 0   |
| 5   | 47.4 | ±0.41 | ±0.41 | ±0.82 | 0 | 0   |
| 6   | 106.5 | ±0.58 | ±0.58 | ±0.58 | 0 | 0   |

Thus, six eigenvalues of \( C_{ij} \) become as follows:

\[
\begin{align*}
\eta^{(1)} &= C_{11} - C_{12} < C_{44} \quad C_{11} - C_{12} < C_{44} \\
\eta^{(2)} &= C_{11} - C_{12} < C_{44} \quad C_{11} - C_{12} < C_{44} \\
\eta^{(3)} &= C_{11} - C_{12} < C_{44} \quad C_{11} - C_{12} < C_{44} \\
\eta^{(4)} &= C_{11} - C_{12} < C_{44} \quad C_{11} - C_{12} < C_{44} \\
\eta^{(5)} &= C_{11} - C_{12} < C_{44} \quad C_{11} - C_{12} < C_{44} \\
\eta^{(6)} &= C_{11} - C_{12} < C_{44} \quad C_{11} - C_{12} < C_{44} \\
\end{align*}
\]

FIG. 1. Stress–strain curve and change in the eigenvalues of \( B_{ij} \) of fcc Ni and Al under the [001] uniaxial static tension.
the latter corresponds to Poisson’s contraction like isotropic expansion/shrinkage in the lateral direction under constant volume. On the other hand, Pt and Al have the lowest resistance in the shear mode.

Elastic coefficients of bcc metals are shown in Table III. Contrary to the previous fcc case, only Fe has the relation of $C_{11} - C_{12} < C_{44}$ so that the other elements have the lowest eigenvalue of $\eta^{(1)} = \eta^{(2)} = \eta^{(3)} = C_{44}$ in the shear without normal strain components. Table IV shows the eigenvector under a small strain of $\varepsilon_{zz} = 0.001$. They are almost the same as in Table II, except the order in the shear mode. That is, the shear $\Delta \gamma_{xy}$ is always located at the top in the three shear modes, while it is at the bottom in Table II. Although the deformation resistance of $C_{44}$ is the same for the three modes, the $xy$ shear is definitely preferable in bcc metals, while it is not in fcc ones against strain perturbation in the $z$-direction.

The $C_{ij}$ of hcp metals are listed in Table V. Hcp metals have anisotropy about $C_{33}$, $C_{13}$, and $C_{66}$ so that the characteristic equation of the submatrix is

$$
\begin{vmatrix}
C_{11} - \eta & C_{12} & C_{13} \\
C_{12} & C_{11} - \eta & C_{13} \\
C_{13} & C_{13} & C_{33} - \eta
\end{vmatrix} = 0.
$$

(4)

The solution is

$$
\eta = C_{11} - C_{12}, \quad A_1 = \frac{\sqrt{A_1^2 + 8C_{13}^2}}{2},
A_1 = C_{11} + C_{12} + C_{33}, \quad A_2 = C_{11} + C_{12} - C_{33}.
$$

(5)

All hcp elements have the $C_{11} - C_{12} > C_{44}$, $C_{66}$ relation. The eigenvalues and eigenvectors of Zhou’s Mg are shown in Table VI. Here, no strain perturbation is applied in the calculation of the eigenvector; however, the ambiguity for $\Delta \gamma_{yz}$ and $\Delta \gamma_{zx}$ vanishes due to the anisotropy of the hcp structure. The same deformation mode of $(\Delta \varepsilon_{xx}, \Delta \varepsilon_{yy}, \Delta \varepsilon_{zz}) = (1, -1, 0), (1, -1, 2)$, and $(1, 1, 1)$ as isotropic fcc and bcc is obtained for the eigenvalues of Eq. (5). The eigenvector is the same for all other elements in Zhou’s potential. Eigenvectors for $\eta^{(1)}$ and $\eta^{(2)}$ are switched in Liu’s potential, but it might have no physical significance due to the same value of $\eta^{(1)} = \eta^{(2)} = C_{44}$.

III. UNIAXIAL TENSION IN [001] AXIS

Figure 1 shows the change in the stress (thick solid line, right scale) and that in the 5 eigenvalues of $B_{ij}$ (left scale) of fcc Ni and Al under the uniaxial static [001] tension. The calculation is
implemented with $10 \times 10 \times 10$ unit lattices, and the lateral strain $\varepsilon_{xx}$ and $\varepsilon_{yy}$ is controlled to reduce the normal stresses to $|\sigma_{xx}|, |\sigma_{yy}| < 0.1$ [GPa]. $\eta^{(6)} = C_{11} + 2 C_{12}$ shows an extremely high value against the other eigenvalues so that it is omitted in the graph. The stress shows a rather unrealistic curve due to the energy cutoff under unrealistic large strain. The components of the eigenvector could be changed with the loading; however, the deformation mode is labeled by the initial eigenvectors. The “instability” is caused by the change in the other eigenvalues so that it is omitted in the graph. The stress–strain curve shows a rather unrealistic curve due to the energy cutoff under unrealistic large strain. The components of the eigenvector could be changed with the loading; however, the deformation mode is labeled by the initial eigenvectors. The “instability” is caused by the change in the other eigenvalues so that it is omitted in the graph.

IV. UNIAXIAL TENSION IN FCC [111], BCC [110], AND HCP [1010]

We perform the same static calculation in different axes: [111] for fcc, [110] for bcc, and [1010] for hcp. Table VII shows the eigenvalues of $C_{ij}$ of Zhou’s Ni and the corresponding eigenvector without any strain. All other fcc elements of Zhou’s and Voter’s Ni and Al also show the same eigenvector in this crystal orientation at $\varepsilon_{zz} = 0$. The 6 eigenvalues of the $6 \times 6$ matrix $C_{ij}$ in the rotated coordinate are definitely identical to those obtained by the coordinate $\Delta \varepsilon_{zz}$, $\Delta \gamma_{zy}$, and $\Delta \gamma_{yz}$ of hcp Mg under the [0001] uniaxial static tension.

![FIG. 3. Stress–strain curve and change in the eigenvalues of $\Delta \varepsilon_{ij}$ of hcp Mg under the [0001] uniaxial static tension.](image)

TABLE VII: Eigenvalues of $C_{ij}$ of fcc Ni (Zhou’s potential) in the $x[110]$, $y[TT2]$, and $z[111]$ coordinates (unit: GPa) and corresponding eigenvectors.

| Ni   | $\Delta \varepsilon_{xx}$ | $\Delta \varepsilon_{yy}$ | $\Delta \varepsilon_{zz}$ | $\Delta \gamma_{yz}$ | $\Delta \gamma_{xy}$ | $\Delta \gamma_{yx}$ |
|------|-----------------------------|-----------------------------|-----------------------------|----------------------|----------------------|----------------------|
| $\eta^{(1)}$ | 49.8                        | 0                           | 0                           | 0.82                 | 0.58                 |                      |
| $\eta^{(2)}$ | 57.2                        | 0.23                        | -0.23                       | 0.94                 | 0.58                 | 0.58                 |
| $\eta^{(3)}$ | 124.6                       | 0                           | 0                           | 0.58                 | 0.58                 | 0.58                 |
| $\eta^{(4)}$ | 216.9                       | -0.67                       | 0.67                        | 0.33                 | 0                    | 0                    |
| $\eta^{(5)}$ | 249.3                       | -0.41                       | -0.41                       | 0.82                 | 0                    | 0                    |
| $\eta^{(6)}$ | 540.4                       | -0.58                       | -0.58                       | -0.58                | 0                    | 0                    |

The results for bcc Fe, Mo, and Ta are shown in Fig. 2. W is similar to Mo and omitted to compare Fe of Zhou and FS. Before the loading, the shear modes are lowest in Mo, Ta, and W; however, the instability is caused by the $(\Delta \varepsilon_{xx}, \Delta \varepsilon_{yy}, \Delta \varepsilon_{zz}) = (1, -1, 2)$ mode in all elements and potential type. Contrary to the previous fcc case, this mode may cause phase transformation since the unstable deformation occurs simultaneously in three normal directions. The unstable point coincides with the stress peak. The corresponding eigenvector at the unstable strain is of $(\Delta \varepsilon_{xx}, \Delta \varepsilon_{yy}, \Delta \varepsilon_{zz}) = (-1, 1, 2)$ in (1, 1, 4) type, Fe(0.39, 0.39, -0.84), Mo(0.24, 0.24, -0.94), Ta(-0.43, -0.43, 0.80), W(-0.26, -0.26, 0.93) for Zhou’s potential, while Fe(−0.32, −0.32, 0.89) for FS potential. Here, the absolute sign and the magnitude of the strain components do not have any physical significance due to the arbitrary sign of the eigenvector normalized as $\sqrt{\Delta \varepsilon_{xx}^2 + \cdots + \Delta \gamma_{xy}^2} = 1$.
FIG. 4. Stress–strain curve and change in the eigenvalue of $B^i_{ij}$ of fcc Ni and Al under the [111] uniaxial static tension.

transformation of the 4th order tensor by $C'_{ijkl} = C_{pqrs}R_{ip}R_{jq}R_{jr}R_{ls}$, where $R_{ij} = e'_i \cdot e_j$ is the rotation tensor and $e_i, e'_i$ is the basis vector of the Cartesian coordinate. Here, we try to transform the previous mode of $(\Delta \varepsilon_{xx}, \Delta \varepsilon_{yy}, \Delta \varepsilon_{zz}) = (1, -1, 0)/\sqrt{2}$ in the [100], [010], [001] coordinates by the rotation tensor as follows:

$$[\Delta \varepsilon'_{ij}] = [\Delta \varepsilon_{ij} R_0 R_0] = \begin{bmatrix} 0 & \frac{1}{\sqrt{6}} & -\frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{6}} & 0 & 0 \\ -\frac{1}{\sqrt{3}} & 0 & 0 \end{bmatrix} \begin{bmatrix} \Delta \varepsilon_{xx} \\ \Delta \varepsilon_{yy} \\ \Delta \varepsilon_{zz} \end{bmatrix}. \quad (6)$$

FIG. 5. Schematic of unstable modes in the (a) fcc [111], (b) bcc [110], and (c) hcp [010] tension.
TABLE VIII. Eigenvalues of $C_{ij}$ of bcc Fe, Mo, and Ta (Zhou’s potential) in the $x[110]$, $y[001]$, and $z[110]$ coordinates (unit: GPa) and the corresponding eigenvectors.

|       | Fe $\Delta\varepsilon_{xx}$ | $\Delta\varepsilon_{yy}$ | $\Delta\varepsilon_{zz}$ | $\Delta\gamma_{yz}$ | $\Delta\gamma_{zx}$ | $\Delta\gamma_{xy}$ | Mo $\Delta\varepsilon_{xx}$ | $\Delta\varepsilon_{yy}$ | $\Delta\varepsilon_{zz}$ | $\Delta\gamma_{yz}$ | $\Delta\gamma_{zx}$ | $\Delta\gamma_{xy}$ | Ta $\Delta\varepsilon_{xx}$ | $\Delta\varepsilon_{yy}$ | $\Delta\varepsilon_{zz}$ | $\Delta\gamma_{yz}$ | $\Delta\gamma_{zx}$ | $\Delta\gamma_{xy}$ |
|-------|-----------------------------|---------------------------|---------------------------|---------------------|---------------------|---------------------|-----------------------------|---------------------------|---------------------------|---------------------|---------------------|---------------------|-----------------------------|---------------------------|---------------------------|---------------------|---------------------|---------------------|
| $\eta^{(1)}$ | 47 0 0 0 0 1 0 0 0 | 113 0 0 0 0 0 | 53 0 0 0 0 0 |
| $\eta^{(2)}$ | 94 0.4 0.4 0 0 0 | 113 0 0 0 | 82 0 0 0 0 0 |
| $\eta^{(3)}$ | 117 0 0 0 0 0 | 145 0 0 0 | 82 0 0 0 |
| $\eta^{(4)}$ | 233 0.7 0 0 0 0 | 290 0.4 0 0 | 164 0 0 0 |
| $\eta^{(5)}$ | 501 0.6 0 0 0 0 | 790 0.6 0 0 | 577 0 0 0 |

Although the number of $\Delta\varepsilon_{xy} = 1/\sqrt{6} = 0.41$ and $\Delta\varepsilon_{zx} = -1/\sqrt{3} = -0.58$ may have some relation with that in Table VII, the transformed eigenvector never matches any mode so that the eigenvectors depend on the coordinate. The mode of $\eta^{(1)}$ in Table VII corresponds to the shear of $\Delta\varepsilon_{xz}$ and that of $\eta^{(2)}$ corresponds to the shear of $\Delta\varepsilon_{yz}$ since the eigenvectors approach $\Delta\varepsilon_{xz} = 1$ and $\Delta\varepsilon_{yz} = 1$ under tension. Figure 4 shows the change in the stress and eigenvalues of Ni and Al under the [111] static tension. Except Voter’s Al, all fcc elements show the instability of $\Delta\gamma_{yz}$ and $\Delta\gamma_{zx}$ dominant shear modes. The eigenvectors at the instability point are $(\Delta\varepsilon_{xx}, \Delta\varepsilon_{yy}, \Delta\gamma_{yz}, \Delta\gamma_{zx}) = (-0.01, 0.01, 1.0)$ and $(\Delta\gamma_{yz}, \Delta\gamma_{zx}) = (1.0, 0.02)$ for Zhou’s Ni. Figure 5 indicates the unit lattices for the fcc [111], bcc [110], and hexagonal prism of hcp under $z = [1010]$ tension. As shown in Fig. 5(a), these shear modes of fcc correspond to the atom migration of partial dislocation. The shear modes of $\Delta\gamma_{yz}$ and $\Delta\gamma_{zx}$ in the previous [0001] hcp tension in Fig. 3 also correspond to similar atom migration. That is, the unstable mode coincides with the atom migration direction on the slip plane, in the case of tension normal...
to the slip plane. Returning to Fig. 4(d), the constant volume mode of $(\Delta \epsilon_{xx},\Delta \epsilon_{yy},\Delta \epsilon_{zz}) = (-1, -1, 2)$ rapidly drops in the Voter’s Al and reaches $\eta < 0$ before these shear modes on the slip plane. This tendency is the same as the previous [001] tension of Fig. 1(d). Voter’s Al might be rather “isotropic” in deformation resistance compared to the other fcc elements.

Table VIII shows the eigenvalues and eigenvectors of bcc Fe, Mo, and Ta of Zhou’s potential in the $x$ [T10], $y$ [001], and $z$ [110] coordinates. W shows the same order in the mode as Ta, and the FS potential is the same as Zhou’s Fe. Mo shows the same lowest mode of $\Delta \gamma_{yy}$ and $\Delta \gamma_{zz}$, while Fe, Ta, and W show the lowest in $\Delta \gamma_{zz}$. Despite this difference at $\epsilon_{zz} = 0$, the first instability is caused by the $\Delta \gamma_{xx}$ mode in all elements and potential, as shown in Fig. 6 (W is omitted). This mode corresponds to the atom migration on the slip plane normal to tension, as schematically shown in Fig. 5(b). We also refer to that the stress–strain peak coincides with the point where $\eta^{(2)}$ becomes negative, under this “static” condition.

Finally, the eigenvalues and eigenvectors of $C_{ij}$ of Zhou’s hcp elements in the $x$ [T2T0], $y$ [000T], and $z$ [T10] coordinates are listed in Table IX. The eigenvector is the same for all the elements including Liu’s Mg. That is, all hcp elements show the lowest mode in $\Delta \gamma_{yy}$ and $\Delta \gamma_{zz}$ in this coordinate before tension. However, the instability is caused by the $(\Delta \epsilon_{xx}, \Delta \epsilon_{yy}, \Delta \epsilon_{zz}) = (1, 0, -1)$ mode in Zhou’s potential, as shown in Fig. 7(a); while the eigenvector changes to $(\Delta \epsilon_{xx}, \Delta \epsilon_{yy}, \Delta \epsilon_{zz}) = (-0.03, 0.34, -0.94)$ at the instability point. This mode may correspond to the deformation on the pyramidal plane, as schematically illustrated in Fig. 5(c). Zhou’s other elements show a similar change as in Fig. 7(a). Liu’s Mg shows simultaneous instability of $(\Delta \epsilon_{xx}, \Delta \epsilon_{yy}, \Delta \epsilon_{zz}) = (0.34, -0.07, -0.94)$ and $\Delta \gamma_{yz}$ shear, as shown in Fig. 7(b). The former also may reflect the pyramidal plane slip. The latter represents the shear parallel to the prismatic plane, which is normal to the tensile direction.

The eigenvalues of Liu’s Mg show a discontinuous curve, especially in Fig. 7(b). The cusp of $\eta^{(1)}$ definitely corresponds to the change in the number of surrounding atoms within the cutoff radius; that is, the eigenvalue rapidly drops just before the top and bottom neighbor atoms go out of the cutoff sphere by tension. Then, the eigenvalue recovers with fewer local density $\rho$ and corresponding embedding energy $F(\rho)$ given by the spline function. Liu’s EAM also represents the 2-body pair potential $\phi(r)$ and the contribution of atomic density $\rho(r)$ by the spline function so that it is sensitive against the change in the surrounding atoms. Voter’s EAM also uses a spline function for $F(\rho)$ so that we can see the same tendency in Fig. 1(d).

V. CONCLUSION

Static calculations on the eigenvalues and eigenvectors of a $6 \times 6$ matrix of atomic elastic stiffness, $B_{ij}^{xx} = \Delta \sigma_{ij}^{xx}/\Delta \epsilon_{ij}$, are implemented for fcc, bcc, and hcp elements with different EAM potentials. First, the eigenvalues and eigenvectors of the elastic coefficients $C_{ij}$ are discussed as the characteristics before tension. The isotropic fcc and bcc have the eigenvalues of double root $C_{11} - C_{12}$, triple root $C_{44}$, and $C_{11} + 2C_{12}$. The corresponding eigenvectors are constant volume modes, $(\Delta \epsilon_{xx}, \Delta \epsilon_{yy}, \Delta \epsilon_{zz}) = (a \pm 1, a \pm 1, 0)$ and $(a \pm 1, a \pm 1, 0)$ for the double root $C_{11} - C_{12}$, each shear $\Delta \gamma_{yz}, \Delta \gamma_{xz}, \Delta \gamma_{xy}$ for triple root $C_{44}$, and dilatancy mode $\Delta \epsilon_{xx} = \Delta \epsilon_{yy} = \Delta \epsilon_{zz}$ for $C_{11} + 2C_{12}$. Anisotropic hcp also shows the same modes. Then, the eigenvalues and eigenvectors of $B_{ij}^{xx}$ (except the $a_3$ related term) are discussed under a static uniaxial tension of fcc [001], bcc [001], and hcp [000]. Fcc elements basically show the instability for the mode of $(\Delta \epsilon_{xx}, \Delta \epsilon_{yy}, \Delta \epsilon_{zz}) = (a, a, 0)$, which leads to proportional expansion/shrinkage in the lateral direction. Bcc shows the instability for the mode of

![FIG. 7](image-url) Stress–strain curve and change in the eigenvalue of $B_{ij}^{xx}$ of hcp Mg under the [T10] uniaxial static tension.
Hcp shows the instability of \( \Delta \gamma_{yz} \) and \( \Delta \gamma_{zx} \) shear, which reflects the atom migration on the basal slip plane. Another calculation of the uniaxial tension for fcc [111], bcc [110], and hcp [010] reveals that the instability changes to shear mode on the slip plane in fcc and bcc. Hcp also changes its mode to constant volume mode and shear; the former may reflect the deformation on the pyramidal plane, and the latter may reflect the deformation on the prismatic plane.

Due to the potential problem and static analysis, the obtained results may not have significance for real material behaviors; however, the present paper could be a milestone for the precise discussion by ab initio density functional theory calculation (revision of our previous report\(^1\)) or for the basic knowledge against complicated local phenomena in molecular dynamics simulations.

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