

Self-interstitial configuration in molybdenum studied by modified analytical embedded atom method

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Abstract. The stability of various atomic configurations containing a self-interstitial atom (SIA) in a model representing Mo has been investigated using the modified analytical embedded atom method (MAEAM). The lattice relaxations are treated with the molecular dynamics (MD) simulation at absolute zero of temperature. Six relatively stable self-interstitial configurations and formation energies have been described and calculated. The results indicate that the [1 1 1] dumbbell interstitial S_{111} has the lowest formation energy, and in ascending order, the sequence of the configurations is predicted to be S_{111} , C, S_{110} , T, S_{001} and O. From relaxed displacement field up to the fifth-NN atoms of six configurations, we know that the relaxed displacements depend not only on separation distances of the NN atoms from the defect centre but also strongly on the direction of the connected line between the NN atoms and the defect centre. The equilibrium distances between two nearest atoms in the core of the S_{111} , C, S_{110} , T, S_{001} and O configurations are $0.72a$, $0.72a$, $0.71a$, $0.72a$, $0.70a$ and $0.70a$, respectively.

Keywords. Molybdenum; self-interstitial; modified analytical embedded atom method; molecular dynamics.

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1. Introduction

In order to design and obtain desired properties of modern materials, a thorough understanding of the material microstructure is necessary. Although the rapid improvement and development of experimental tools in recent years, e.g., the scanning tunneling microscope (STM), the field ion microscope (FIM), the high-resolution transmission electron microscope (HRTEM), etc., have significantly improved the prospects for directly observing the structures of crystal defects at atomic level,

many details of these structures remain beyond the scope of these tools [1]. Furthermore, it is not easy to experimentally determine precisely the atomic quantities such as the formation energy of an interstitial or a single vacancy, since these quantities are affected by the local environment (for instance, the impurities) of the defect which is very difficult to probe [2]. Therefore, atomistic simulations based on realistic physical models are becoming powerful supplement to the current experimental methods.

Despite a great body of existing work, there is still uncertainty in understanding the structure and basic properties of SIA defects in bcc molybdenum. For examples, Xu and Moriarty [1], using multi-ion interatomic potentials derived from first-principles generalized pseudopotential theory, predicted the [1 1 0] dumbbell as the most stable SIA configuration in Mo, while Han *et al* [3] and Nguyen-Manh *et al* [4], using *ab initio* calculation, found that the [1 1 1] configuration had the lowest formation energy. Thus it is necessary to investigate the issue with other theoretical approaches. In this paper, six self-interstitial configurations T, O, C, S₀₀₁, S₁₁₀ and S₁₁₁ in Mo have been investigated by the modified analytical embedded atom method (MAEAM), which was developed by Zhang *et al* [5] from initial EAM [6–8] and AEAM [9–11] by adding a modified term to describe the energy deviation from the linear superposition of atomic electronic density in crystal and has been used successfully in our previous paper to investigate the interface [12,13], grain boundary [14,15], surface adsorption [16] and vacancies [17–19]. The results that the formation energy of the self-interstitial configuration increases for S₁₁₁, C, S₁₁₀, T, S₀₀₁ and O successively are consistent with *ab initio* calculation [3,4]. Furthermore, the equilibrium distances between two nearest atoms in the core of the S₁₁₁, C, S₁₁₀, T, S₀₀₁ and O configurations are 0.72a, 0.72a, 0.71a, 0.72a, 0.70a and 0.70a, respectively. The detailed relaxed displacement fields up to the fifth nearest-neighbour (NN) atoms show that the relaxed displacements depend not only on separation distances of the NN atoms from the defect centre but also strongly on the direction of the connected line between the NN atoms and the defect centre.

2. Methodology

2.1 MAEAM

In MAEAM, the total energy E_{total} of a crystal is expressed as [5]

$$E_{\text{total}} = \sum_i F(\rho_i) + \frac{1}{2} \sum_i \sum_{j(\neq i)} \phi(r_{ij}) + \sum_i M(P_i), \quad (1)$$

$$\rho_i = \sum_{j(\neq i)} f(r_{ij}), \quad (2)$$

$$P_i = \sum_{j(\neq i)} f^2(r_{ij}), \quad (3)$$

where $F(\rho_i)$ is the energy to embed an atom in site i with electron density ρ_i , which is given by a linear superposition of the spherical averaged atomic electron density of other atoms $f(r_{ij})$, r_{ij} is the separation distance of atom j from atom i , $\phi(r_{ij})$ is the pair potential between atoms i and j , and $M(P_i)$ is the modified term, which describes the energy deviation from the linear superposition. Embedding function $F(\rho_i)$, pair potential $\phi(r_{ij})$, modified term $M(P_i)$ and atomic electron density $f(r_{ij})$ take the following forms [20,21]:

$$F(\rho_i) = -F_0 \left[1 - n \ln \left(\frac{\rho_i}{\rho_e} \right) \right] \left(\frac{\rho_i}{\rho_e} \right)^n, \quad (4)$$

$$\phi(r_{ij}) = k_0 + k_1 \left(\frac{r_{ij}}{r_{1e}} \right)^2 + k_2 \left(\frac{r_{ij}}{r_{1e}} \right)^4 + k_3 \left(\frac{r_{1e}}{r_{ij}} \right)^{12}, \quad (r_{ij} \leq r_{2e}), \quad (5)$$

$$M(P_i) = \alpha \left(\frac{P_i}{P_e} - 1 \right)^2 \exp \left[- \left(\frac{P_i}{P_e} - 1 \right)^2 \right], \quad (6)$$

$$f(r_{ij}) = f_e \left(\frac{r_{1e}}{r_{ij}} \right)^6, \quad (7)$$

where the subscript e denotes equilibrium state and r_{1e} is the first nearest-neighbour distance at equilibrium. In this paper, the atomic electron density at equilibrium state f_e is chosen as [20]

$$f_e = \left(\frac{E_c - E_{1f}}{\Omega} \right)^{3/5}, \quad (8)$$

where $\Omega = a^3/2$ is the atomic volume of a metal with bcc structure.

The seven parameters F_0 , n , k_0 , k_1 , k_2 , k_3 and α in eqs (4)–(6) can be determined by fitting the cohesion energy E_c , the mono-vacancy formation energy E_{1f} (the definition of E_{1f} is that $E_{1f} = E_t^v - (E_t - E_c)$, where E_t^v and E_t are the total energies of the lattices with and without a vacancy and E_c is the cohesion energy and compensates for the missing atom), the lattice constant a , and elastic constants C_{11} , C_{12} and C_{44} . According to the principle that the energy versus separation distance curve fits the Rose equation [22], we get

$$n = \sqrt{\frac{\Omega(C_{11} + 2C_{12})(C_{11} - C_{12})}{(216E_{1f}C_{44})}}, \quad (9)$$

$$\alpha = \frac{\Omega(C_{12} - C_{44})}{32} - \frac{n^2 F_0}{8}, \quad (10)$$

$$F_0 = E_c - E_{1f}. \quad (11)$$

The parameters of the potential energy k_0 , k_1 , k_2 and k_3 can be calculated with the following formulae for bcc metals [23]:

$$k_0 = -\frac{E_{1f}}{7} - \frac{\Omega(-57111C_{11} + 57111C_{12} + 51519C_{44})}{471800}, \quad (12)$$

$$k_1 = \frac{\Omega(-52563C_{11} + 52563C_{12} + 33327C_{44})}{269600}, \quad (13)$$

$$k_2 = \frac{\Omega(147456C_{11} - 147456C_{12} - 59049C_{44})}{1887200}, \quad (14)$$

$$k_3 = \frac{1536\Omega(-C_{11} + C_{12} + 4C_{44})}{412825}. \quad (15)$$

According to Zhang and Ouyang, the pair-potential $\phi(r_{ij})$ represented by eq. (5) is useable only if the separated distance between atoms is shorter than the second neighbour distance r_{2e} and should be substituted by the following cubic spline function (termed as a cut-off potential) [20]

$$\phi(r_{ij}) = l_0 + l_1 \left(\frac{r_{ij}}{r_{2e}} - 1 \right) + l_2 \left(\frac{r_{ij}}{r_{2e}} - 1 \right)^2 + l_3 \left(\frac{r_{ij}}{r_{2e}} - 1 \right)^3, \quad (16)$$

$(r_{2e} < r_{ij} \leq r_c).$

Four parameters l_0 , l_1 , l_2 , l_3 and cut-off radius r_c are taken as

$$l_0 = k_0 + k_1 s^2 + k_2 s^4 + k_3 s^{-12}, \quad (17)$$

$$l_1 = 2k_1 s^2 + 4k_2 s^4 - 12k_3 s^{-12}, \quad (18)$$

$$l_2 = -\frac{2l_1}{(\gamma - 1)} - \frac{3l_0}{(\gamma - 1)^2}, \quad (19)$$

$$l_3 = \frac{l_1}{(\gamma - 1)^2} + \frac{2l_0}{(\gamma - 1)^3}, \quad (20)$$

$$r_c = r_{2e} + 0.75(r_{3e} - r_{2e}), \quad (21)$$

where r_{2e} and r_{3e} are the second and third neighbour distances at equilibrium, $s = r_{2e}/r_{1e}$ and $\gamma = r_c/r_{2e}$.

Inserting physical parameters such as lattice constant a [23], cohesion energy E_c [24], mono-vacancy formation energy E_{1f} [25] and elastic constants C_{11} , C_{12} and C_{44} [26] (all these are listed in table 1 for convenience) into eqs (8)–(15) and then into eqs (17)–(20), we can obtain the model parameters f_e , F_0 , n , α , k_i and l_i ($i = 0, 1, 2, 3$) for Mo, which are listed in table 2.

Table 1. The input physical parameters for Mo.

| a (Å) | E_c (eV) | E_{1f} (eV) | C_{11} (eV/nm ³) | C_{12} (eV/nm ³) | C_{44} (eV/nm ³) |
|---------|------------|---------------|--------------------------------|--------------------------------|--------------------------------|
| 3.1468 | 6.82 | 3.10 | 2.87 | 1.05 | 0.69 |

2.2 Computational procedure

A system which consists of an outer region and an inner region containing a SIA at the centre is used in the simulation. The atoms in the outer region are assumed to be fixed at their perfect lattice sites and are used as boundary to ensure that each atom in the simulation region has a complete set of neighbours within the range of interatomic potential. The atoms in the inner simulation region are fully relaxed till the minimum energy is reached. The lattice relaxations resulted from the existence of the SIA are treated with the MD simulation [20,21]. The force applied to the i th atom from the other atoms is calculated by

$$f_i^\alpha = -\frac{\partial E_i}{\partial r_{ij}^\alpha} = -\left[F'(\rho_i) \sum_{j(\neq i)} f'(r_{ij}) \frac{r_{ij}^\alpha}{r_{ij}} + \frac{1}{2} \sum_{j(\neq i)} \phi'(r_{ij}) \frac{r_{ij}^\alpha}{r_{ij}} + 2M'(P_i) \sum_{j(\neq i)} f(r_{ij}) f'(r_{ij}) \frac{r_{ij}^\alpha}{r_{ij}} \right], \quad (22)$$

where the superscript α (denotes x , y or z) in f_i^α and r_{ij}^α represents the α th component of the force (f_i) and the separation distance (r_{ij}) of atom j from atom i . $E_i = F(\rho_i) + \frac{1}{2} \sum_{j(\neq i)} \phi(r_{ij}) + M(P_i)$ is the energy contribution from atom i and eq. (1) becomes

$$E_{\text{total}} = \sum_i E_i. \quad (23)$$

The interstitial formation process is defined here as the creation of an interstitial structure from a corresponding perfect crystal lattice having the same number of normal atoms [27]. The relaxed SIA formation energy E_f^I is defined as [28]

$$E_f^I = E_t^I - (E_t + E_c), \quad (24)$$

where E_t^I and E_t are the energies of the relaxed lattices with and without a SIA and E_c is the cohesion energy and counteracts the adding interstitial atom.

3. Results and discussion

3.1 Unrelaxed

An interstitial atom can position in a crystal in two ways: (1) normal atoms at their perfect lattice sites and the interstitial atom lying in interstitial position of

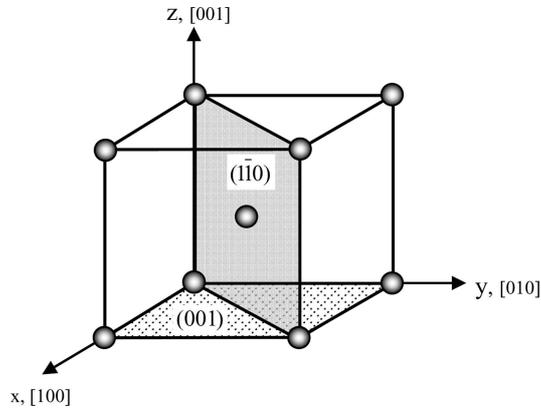


Figure 1. A single SIA or one of the dumbbell atoms assumed to move on the representative symmetrical plane (001) or $(1\bar{1}0)$ of bcc crystal.

the coordination polyhedrons of the crystallite, (2) dumbbell interstitial, that is, two atoms are symmetrically split in one direction sharing a vacant normal lattice site. From the analysis of the resultant force, we know that these interstitial defects should be distributed on the symmetrical planes of the crystal, that is $\{100\}$ and $\{110\}$ for cubic structure. As is shown in figure 1, a single SIA or one of the dumbbell atoms with position coordinate $(x, y, 0)$ or $(x, y \equiv x, z)$ is assumed to move at intervals of 0.05 \AA on the representation plane (001) or $(1\bar{1}0)$, and at each position the interstitial energy is calculated, The minimum values of the energy and the corresponding positional coordinates are listed in table 3 and shown schematically in figure 2.

We can see that these relatively stable self-interstitial positions are tetrahedron, octahedron and crowdion single interstitial sites, and $[001]$, $[110]$ and $[111]$ dumbbell interstitial sites. These sites locate either in a large ‘open space’ or at the higher symmetry element positions of the lattice. To describe conveniently, we abbreviate these six positions as T, O, C, S_{001} , S_{110} and S_{111} , respectively. The crowdion is lying in the closest packed row of the lattice and a $[hkl]$ dumbbell (or split) interstitial lies in a position in which the interstitial and another atom are arranged symmetrically in the $[hkl]$ direction sharing and slightly displaced from a vacant normal lattice site. Johnson *et al* [31] have also demonstrated its stability in a lattice model rather similar to ours. The distances of the T, O and C SIA separated from their first-NN atoms are $0.56a$, $0.50a$ and $0.43a$ and the lengths of the S_{001} , S_{110} and S_{111} dumbbells are $0.68a$, $0.65a$ and $0.59a$, respectively.

3.2 Relaxed

The calculated interstitial formation energies after relaxation are listed in table 3 along with *ab initio* calculation data [3,4] for comparison. The calculated interstitial formation energies are generally lower than the *ab initio* calculations and may be resulted from simplifications of the last two terms on the right-hand side

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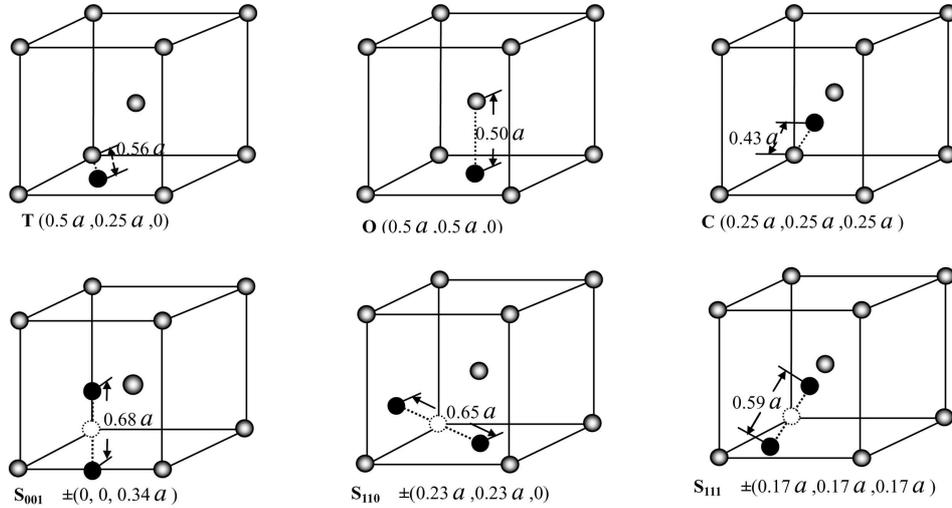


Figure 2. Schematic figures of the six relatively stable self-interstitial configurations for Mo.

of total energy expression (1), i.e., pair potential $\phi(r_{ij})$ and the modified term $M(P_i)$. The pair-potential $\phi(r_{ij})$ between atoms i and j is not included while the separation distances of atoms j from atom i are larger than the cut-off radius $r_c = r_{2e} + 0.75(r_{3e} - r_{2e})$ selected in eq. (21). The modified term $M(P_i)$ is added to describe the energy contribution from a non-linear superposition of the spherical averaged atomic electron density of other atoms $f(r_{ij})$. A complete form of a non-linear superposition of the spherical averaged atomic electron density of other atoms $f(r_{ij})$ should be $P_i = \sum_{j \neq i} [f^2(r_{ij}) + f^3(r_{ij}) + \dots]$. However, as presented in eq. (3), $P_i = \sum_{j(\neq i)} f^2(r_{ij})$, only the second-order term is considered and the terms corresponding to the higher-order have been neglected. If a relatively larger cut-off radius and more higher-order terms are used in eqs (21) and (3), the higher interstitial formation energies can be obtained with the MAEAM interatomic potentials. Although the present results are lower than the *ab initio* results, as shown in figure 3 for the formation energies of the six SIA configurations relative to the lowest-energy configuration S_{111} , the sequences of the six configurations in energetic order are identical. From the minimization of the formation energy, we know that the preferred interstitial configurations are S_{111} , C, S_{110} , T, S_{001} and O successively.

The formation of interstitial defect will result in a rearrangement of the matrix atoms in the vicinity of the interstitial. The lattice distortion is determined by an iteration process minimizing the energy. The calculated equilibrium positions of the SIA for the six interstitial configurations are also given in table 3. The equilibrium distances between two nearest atoms in the core of the S_{111} , C, S_{110} , T, S_{001} and O configurations are $0.72a$, $0.72a$, $0.71a$, $0.72a$, $0.70a$ and $0.70a$ respectively. The displacement fields around the SIA up to the fifth-NN atoms are listed in table 4 for T, O, C, S_{111} , S_{110} and S_{001} . For the single interstitials and the dumbbells, the distribution of the same NN atoms is symmetrical about the centre of the interstitial

Table 2. The MAEAM model parameters for Mo, F_0 , α , k_i , l_i ($i = 0, 1, 2, 3$) in eV.

| f_e | F_0 | n | α | k_0 | k_1 | k_2 | k_3 | l_0 | l_1 | l_2 | l_3 |
|---------|-------|---------|----------|--------|---------|--------|----------|----------|--------|---------|---------|
| 0.42343 | 3.72 | 0.55229 | 0.033441 | 1.8157 | -4.1996 | 1.8792 | 0.054491 | -0.43316 | 2.0482 | 0.27875 | -7.6724 |

Table 3. The formation energy and the corresponding positions of a single or dumbbell interstitial on the (001) or (1 $\bar{1}$ 0) plane. D represents the distances between the single SIA and its first NN atoms or the lengths of dumbbell interstitials.

| Plane | Sites | Unrelaxed | | | | Relaxed | | | |
|-----------------|------------------|---------------|-----------------------|--------|---------------------|-----------------------|---------------------|--|--|
| | | E_{if} (eV) | Positions (a) | $D(a)$ | E_{if} (eV) | Positions (a) | $D(a)$ | | |
| (001) | T | 48.66 | (0.5,0.25,0) | 0.56 | 6.74 | (0.5,0.25,0) | 0.72 | | |
| | O | 91.15 | (0.5,0.5,0) | 0.50 | 8.20 [3], 8.401 [4] | (0.5,0.5,0) | 0.70 | | |
| | C | 467.02 | (0.25,0.25,0.25) | 0.43 | 8.86 [3], 9.067 [4] | (0.25,0.25,0.25) | 0.72 | | |
| (1 $\bar{1}$ 0) | S ₀₀₁ | 11.54 | $\pm(0,0,0.34)$ | 0.68 | 7.34 [3], 7.419 [4] | $\pm(0,0,0.35)$ | 0.70 | | |
| | S ₁₁₀ | 15.26 | $\pm(0.23,0.23,0)$ | 0.65 | 6.87 | $\pm(0.25,0.25,0)$ | 0.71 | | |
| | S ₁₁₁ | 26.26 | $\pm(0.17,0.17,0.17)$ | 0.59 | 8.77 [3], 9.004 [4] | $\pm(0.21,0.21,0.21)$ | 0.7 [29], 0.75 [30] | | |
| | | | | | 7.51 [3], 7.581 [4] | | 0.72 | | |

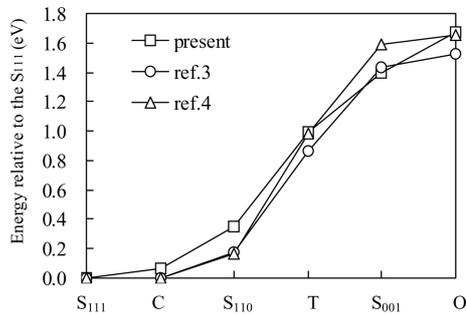


Figure 3. Formation energies of the six SIA configurations relative to the S₁₁₁.

defects. So only the displacements of one atom on the symmetrical position are given. The negative values refer a motion along negative direction of axis. It is noted that the displacements of NN atoms to a SIA are very large compared to those to a vacancy in ref. [1]. This is because adding a SIA into normal matrix will result in a large decrease in interatomic distance and thus a large increase in the acting force, while removing an atom from normal matrix will result in a slight change in the acting force.

Figure 4 shows the schematic picture of the relaxed displacements lying on the $(1\bar{1}0)$ plane up to the fifth-NN atoms of the SIA O and C sites, and core of the dumbbell S₁₁₁, S₁₁₀ and S₀₀₁. The gray and black balls represent normal matrix Mo atoms and the SIA, respectively. The arrows represent the directions and magnitudes (enlarged different times) of the movement of these atoms. The third- and fifth-NN atoms are absent for SIA O and C sites, respectively, since they do not lie on the $(1\bar{1}0)$ plane.

From table 4 and figure 4, we can see that the relaxed displacements depend not only on separation distances of the NN atoms from the SIA but also strongly on the direction of the connected line between the NN atoms and the self-interstitial centre. For the occupying high-symmetry O site, each atom in the vicinity of SIA moves approximately along the connected line between the atom and the SIA. Up to the fifth-NN atoms, the movements are outward the SIA, except for the third-NN atoms moving toward the SIA. The further the NN atoms from the O site SIA are, the smaller the relaxed displacements are. A relatively large relaxed displacements occur for atoms aligned along the $[001]$ direction containing SIA. Similar relaxed configurations are obtained for C and S₁₁₁, the deformation is largely confined to a single string of atoms running in the $[111]$ direction. The same result was reported in ref. [4]. The relatively larger displacements occurred for atoms lying on the $[111]$ string are given in italics for convenience in table 4. Similar symmetry and relaxed structures for C and S₁₁₁ result in a nearly equal formation energy as can be seen in figure 3. For S₁₁₀ and S₀₀₁, the relaxed displacement fields of the NN atoms are symmetric about the dumbbell. Up to the fifth-NN atoms, the movements are outward except the second-NN atoms of S₁₁₀ moving inward.

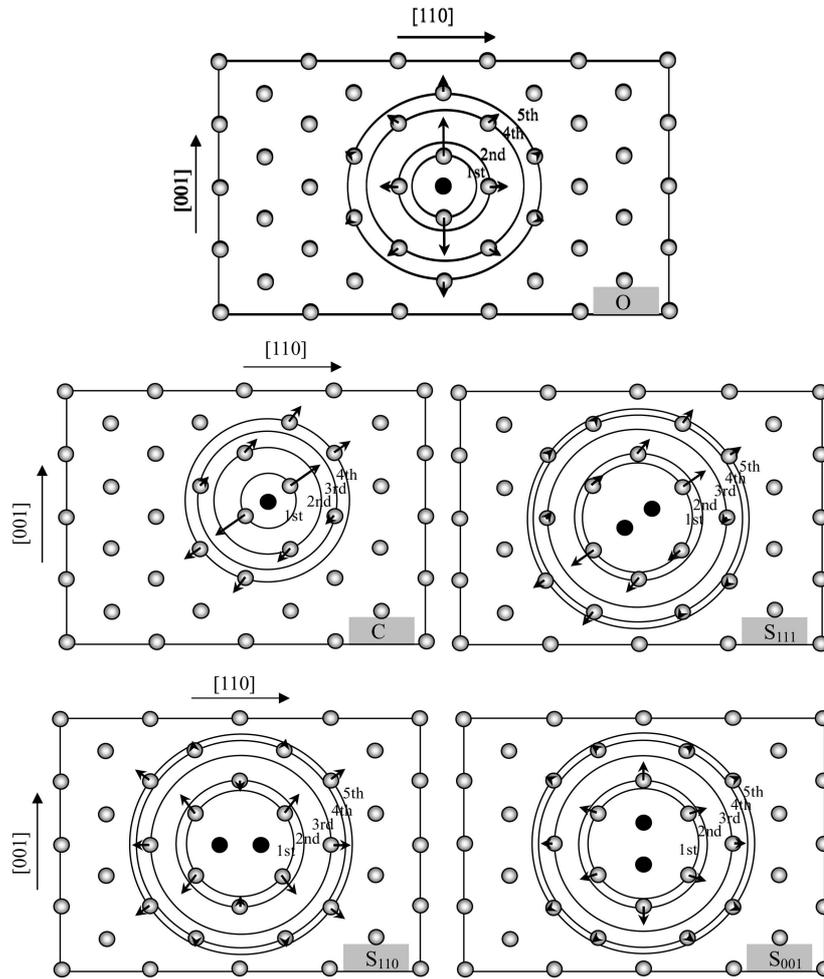


Figure 4. The relaxed atomic displacements lying on $(1\bar{1}0)$ plane in the vicinity of the SIA. The gray and black balls represent normal matrix Mo atoms and the SIA, respectively. The arrows represent the displacement directions and magnitudes (enlarged three and six times for the 1st NN atoms and the further NN atoms in O, S_{110} and S_{001} , two and eight times for the atoms in and out of the $[111]$ string respectively in C and S_{111}).

4. Conclusions

This paper has mainly been concerned with the stability of various atomic configurations containing a SIA in molybdenum. There are several points of interest to mention. First, the $[111]$ dumbbell interstitial has the lowest formation energy, and in ascending order, the sequence of configurations is predicted to be S_{111} , C, S_{110} ,

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Table 4. The displacement field around the SIA. Δx , Δy and Δz represent the relaxed displacement along x -, y - and z -axes respectively, $\Delta d = \sqrt{(\Delta x)^2 + (\Delta y)^2 + (\Delta z)^2}$ is the total relaxed displacement.

| Interstitial configuration | Nearest neighbours | Initial positions | $\Delta x(a)$ | $\Delta y(a)$ | $\Delta z(a)$ | $\Delta d(a)$ |
|--|--------------------|----------------------|---------------|---------------|---------------|---------------|
| T (0.5,0.25,0) a | 1st | (0,0,0) a | -0.14516 | -0.07868 | 0.00000 | 0.16512 |
| | 2nd | (1,1,0) a | -0.01583 | 0.00616 | 0.00000 | 0.01697 |
| | 3rd | (0,0,1) a | 0.00168 | -0.01036 | -0.02123 | 0.02367 |
| | 4th | (0,1,1) a | -0.02758 | 0.03168 | 0.03028 | 0.05180 |
| | 5th | (0,-1,0) a | -0.01459 | -0.01856 | 0.00000 | 0.02361 |
| O (0.5,0.5,0) a | 1st | (-1,0,0) a | -0.02682 | -0.00076 | 0.00000 | 0.02682 |
| | 1st | (0.5,0.5,0.5) a | 0.00000 | 0.00000 | 0.20163 | 0.20163 |
| | 2nd | (0,0,0) a | -0.03384 | -0.03384 | 0.00000 | 0.04786 |
| | 3rd | (0.5,1.5,-0.5) a | 0.00000 | -0.02965 | 0.00184 | 0.02971 |
| | 4th | (0,0,-1) a | -0.02078 | -0.02078 | -0.01726 | 0.03410 |
| C (0.25,0.25,0.25) a | 5th | (1.5,1.5,0.5) a | 0.00960 | 0.00960 | 0.00483 | 0.01440 |
| | 1st | (0.5,0.5,1.5) a | 0.00000 | 0.00000 | 0.04230 | 0.04230 |
| | 1st | (0.5,0.5,0.5) a | 0.16420 | 0.16420 | 0.16420 | 0.28442 |
| | 2nd | (0,0, a) | 0.01926 | 0.01926 | 0.02456 | 0.03667 |
| | 3rd | (-0.5,-0.5,0.5) a | 0.01160 | 0.01160 | 0.01776 | 0.02418 |
| S ₁₁₁ $\pm(0.17,0.17,0.17)a$ | 4th | (-0.5,-0.5,-0.5) a | -0.08984 | -0.08984 | -0.08984 | 0.15562 |
| | 5th | (0.5,0.5,1.5) a | 0.01700 | 0.01700 | 0.03124 | 0.03941 |
| | 1st | (-1,0,1) a | -0.00680 | -0.00067 | 0.00594 | 0.00906 |
| | 1st | (0.5,0.5,0.5) a | 0.12565 | 0.12565 | 0.12565 | 0.21765 |
| | 2nd | (0.5,0.5,-0.5) a | -0.01719 | -0.01719 | -0.02066 | 0.03191 |
| S ₁₁₀ $\pm(0.23,0.23,0)a$ | 3rd | (0,0,1) a | 0.01776 | 0.01776 | 0.02939 | 0.03864 |
| | 4th | (1,1,0) a | -0.00756 | -0.00756 | -0.01484 | 0.01830 |
| | 5th | (-1,1,0) a | -0.00620 | 0.00620 | 0.00000 | 0.00877 |
| | 4th | (0.5,0.5,1.5) a | 0.01459 | 0.01459 | 0.02708 | 0.03403 |
| | 5th | (0.5,0.5,-1.5) a | -0.00302 | -0.00302 | -0.00667 | 0.00791 |
| S ₁₁₀ $\pm(0.23,0.23,0)a$ | 5th | (0.5,-0.5,1.5) a | 0.00124 | -0.00562 | 0.00696 | 0.00903 |
| | 1st | (1,1,1) a | 0.06178 | 0.06178 | 0.06178 | 0.10700 |
| | 2nd | (1,1,-1) a | -0.00270 | -0.00270 | -0.00410 | 0.00559 |
| | 1st | (0.5,0.5,0.5) a | 0.05421 | 0.05421 | 0.10096 | 0.12676 |
| | 2nd | (0.5,-0.5,0.5) a | -0.00922 | 0.00922 | -0.01436 | 0.01938 |
| | 3rd | (0,0,1) a | 0.00000 | 0.00000 | -0.02914 | 0.02914 |
| | 4th | (1,0,0) a | 0.04080 | 0.00982 | 0.00000 | 0.04198 |
| | 5th | (-1,-1,0) a | 0.01640 | 0.01640 | 0.00000 | 0.02320 |
| | 3rd | (-1,0,-1) a | -0.00725 | 0.01046 | -0.00296 | 0.01306 |
| | 4th | (-1,1,0) a | 0.00000 | 0.00000 | 0.00000 | 0.00000 |
| 5th | (0.5,0.5,1.5) a | 0.00064 | 0.00064 | 0.01706 | 0.01834 | |
| | (-0.5,1.5,0.5) a | -0.00365 | 0.00588 | 0.00105 | 0.00699 | |
| | (0.5,-0.5,1.5) a | -0.00369 | 0.00369 | -0.00003 | 0.00521 | |
| 5th | (1,1,1) a | 0.02603 | 0.02603 | 0.02717 | 0.04576 | |
| | (-1,1,1) a | 0.00064 | -0.00064 | -0.00210 | 0.00229 | |

contd...

Table 4. Contd...

| Interstitial configuration | Nearest neighbours | Initial positions | $\Delta x(a)$ | $\Delta y(a)$ | $\Delta z(a)$ | $\Delta d(a)$ |
|-------------------------------|--------------------|-------------------|---------------|---------------|---------------|---------------|
| S_{001} $\pm(0,0,0.34)a$ | 1st | $(0.5,0.5,0.5)a$ | 0.03178 | 0.03178 | 0.01503 | 0.04738 |
| | 2nd | $(0,0,1)a$ | 0.00000 | 0.00000 | 0.09724 | 0.09724 |
| | | $(1,0,0)a$ | -0.03810 | 0.00000 | 0.00000 | 0.03810 |
| | 3rd | $(0,1,1)a$ | 0.00000 | -0.01455 | -0.00191 | 0.01468 |
| | | $(1,1,0)a$ | 0.01071 | 0.01071 | 0.00000 | 0.01516 |
| 4th | $(0.5,0.5,1.5)a$ | 0.01179 | 0.01179 | 0.01363 | 0.02155 | |
| 5th | $(1.5,0.5,0.5)a$ | 0.00439 | -0.00324 | -0.00153 | 0.00566 | |
| | | $(1,1,1a)a$ | 0.01030 | 0.01030 | 0.00664 | 0.01602 |

T, S_{001} and O. This is in agreement with the *ab initio* calculations. Second, the equilibrium distances between two nearest atoms in the core of the S_{111} , C, S_{110} , T, S_{001} and O configurations are $0.72a$, $0.72a$, $0.71a$, $0.72a$, $0.70a$ and $0.70a$ respectively. Finally, the relaxed displacements depend not only on separation distances of the NN atoms from the SIA but also strongly on the direction of the connected line between the NN atoms and the self-interstitial centre.

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