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# Atomistic simulation of energetic displacement cascades near an Ni–graphene interface

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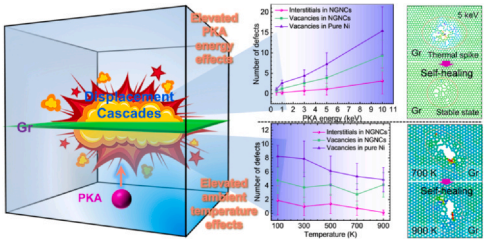
## HIGHLIGHTS

- Ni–graphene nanocomposites may resist irradiation damage for SCWRs.
- Elevated cascade energy could significantly promote the formation of defects.
- Ambient temperature has slight effect on the number of surviving defects.
- Annealing from irradiation and ambient temperature may repair damaged graphene.
- Ni–graphene interfaces exhibit high sink efficiency for irradiation defects.

## GRAPHICAL ABSTRACT

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## ABSTRACT

Ni–graphene nanocomposites have greatly promising applications in supercritical water-cooled reactors due to their outstanding performances. However, many fundamental mechanisms of irradiation behaviors in the composites are still unclear. Here we investigate the displacement cascades near an Ni–graphene interface using atomistic simulations. Different cascade energies and ambient temperatures were introduced to bring out the effect of irradiation. The increasing cascade energy in the interval 0.5–10 keV could significantly promote the formation of defects, while there is slight effect on the number of surviving defects in Ni matrix when adjusting the ambient temperature from 100 K to 900 K. The damaged graphene could be self-healing by the synergistic effects of irradiation annealing and ambient temperature annealing. The interface exhibits high sink efficiency for irradiation defects in all cases. This study provides an important insight into the understanding of the microscopic evolution of defects in cascades for the composites.

## 1. Introduction

Supercritical water-cooled reactors (SCWRs), using supercritical pressure water as a coolant, are believed as one of the promising Gen-IV nuclear energy systems due to the high thermal efficiency and significant plant simplification [1–3]. Faced with the challenge of developing SCWRs, designing irradiation-tolerant materials from the perspective of interface engineering has gradually become a mainstream consensus among the materials community [4–9]. Generally, the interiors of crystalline materials tend to form a mass of point defects (*i.e.*, interstitials and vacancies) under extreme radiation exposure of reactors. Along with elevated temperature, those point defects easily aggregate to form voids, dislocation

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loops, and stacking fault tetrahedra (SFTs), which may threaten service safety of structural materials in the forms of swelling, embrittlement, and hardening [9–13]. Various types of interfaces, including grain boundaries and phase boundaries, can serve as sinks for radiation-induced defects [6,7,9,13]. Consequently, nanostructured materials with high-density interfaces exhibit the ability to significantly alleviate irradiation damage for the advanced fission reactors.

Recently, a new class of nanostructured materials, called metal–graphene (Gr) nanocomposites, have been gradually proven to possess excellent irradiation tolerance by different research groups [14–18], since they are rich in plenty of ultra-high-strength interfaces. Especially, the Ni–Gr nanocomposites (NGNCs), which also have excellent elevated-temperature mechanical properties, high thermal/electrical conductivity, and enhanced corrosion resistance [19–24], become candidate structural materials for SCWRs that urgently need irradiation-tolerant Ni-based materials [25–28]. Several irradiation studies on NGNCs have been carried out [17,29–31]. On the simulation side, it has been demonstrated that Ni–Gr interfaces (NGIs) can attract, absorb, and annihilate interstitials, vacancies, and He atoms/clusters [17,30,31]. Experimentally, NGNCs exhibit less crystal defects (*e.g.*, lattice swelling and stacking faults) and smaller He bubbles than those in pure Ni under energetic ion irradiation [29]. These studies have given researchers greater confidence for the application of NGNCs in the nuclear reactors. Nevertheless, to the best of our knowledge, the study of irradiation damage in NGNCs is still in its infancy, and even many fundamental mechanisms have not been understood comprehensively.

Energetic particles (*e.g.*, fast neutrons and fission fragments) can produce displacements of lattice atoms and introduce many primary knock-on atoms (PKAs) with kinetic energies ranging from a few hundred eV to hundreds of keV, further initiating different levels of displacement cascades [32–34]. Evolution of point defects in cascades has an important influence on the microstructure. Since the whole stage of primary irradiation damage is on the time and space scales of the orders of ps and nm, it is impractical with current experimental techniques to acquire the microscopic information [33]. In recent decades, classical molecular dynamics (MD) has been a powerful method to study the displacement cascades in various materials, due to their ability to provide important insights into the understanding of the creation, mobility, clustering, and interaction of point defects on the dimension of ps-nm [33,35–37].

In the present work, to illuminate the irradiation response of NGNCs, MD simulations were performed to investigate the displacement cascades near an NGI. The evolution of point defects, their stability, and their interaction with the NGI were discussed during displacement cascades depending on ambient temperature and initial PKA conditions [33,34,36,37]. Also, the atom configurations near the NGI related to the radiation environments were compared.

## 2. Simulation methodology

To study the displacement cascades near NGIs, a sandwich-like NGI model with the dimensions of 124.6 × 129.5 × 174.5 Å$^3$ (258,000 atoms) was generated as exhibited in Fig. 1(a). The interactions among C atoms in Gr, the interactions between Ni atoms, and the C–Ni interactions were described by the adaptive intermolecular reactive empirical bond order (AIREBO) potential [38], the embedded atom method (EAM) potential developed by Bonny et al. [39], and the Lennard–Jones potential [40], respectively. The setting of each potential, the optimization and thermal equilibrium of the model, and the identification of interface and bulk regions have been described elsewhere [17]. All simulations were carried out using the parallel MD code LAMMPS [41], and visualizations were rendered with OVITO [42].

Displacement cascades were launched in the model system by a PKA introduced at a certain distance away from the interface, and the PKA was incident perpendicular to the interface (Fig. 1(b)). During cascades, the outer layer with 10 Å thickness was controlled using Nose-Hoover thermostat (NVT ensemble) to dissipate the heat, while other atoms were allowed to move adiabatically using NVE ensemble [17]. The simulations lasted 23 ps. When investigating the influence of PKA energy, the kinetic energy of PKA was selected as 0.5, 1.0, 3.0, 5.0, or 10.0 keV, and the corresponding distance of PKA to the NGI was determined to be 11.0, 15.0, 15.0, 15.0, or 21.1 Å, respectively. These distances can ensure that the center of each cascade is as close to the NGI as possible and defect distribution is approximately symmetrical about the NGI (detailed in Supplementary Material). The thermostat temperature was maintained to 300 K. When investigating the influence of ambient temperature, the thermostat temperature was set to be 100, 300, 500, 700, or 900 K, respectively. The energy of each PKA and the distance of each PKA to the NGI were specified as 5.0 keV and 15.0 Å, respectively. Wigner–Seitz cell method [10,17] was adopted to detect the point defects in the bulk. As a control, the simulation settings of pure Ni for performing cascades were kept consistent with those of NGNCs.

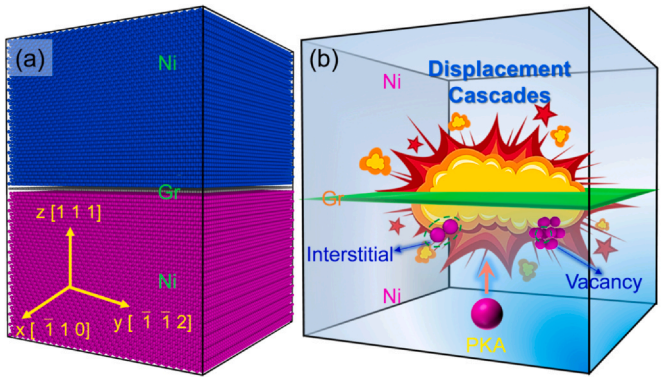


**Fig. 1.** Simulation model. (a) Atomic configuration of NGI. (b) Conceptual schematic of displacement cascades near the NGI.

## 3. Results and discussion

### 3.1. Elevated PKA energy effects on displacement damage

Fig. 2(a) and (b) shows the typical time evolution of the numbers of interstitials and vacancies in the bulk during displacement cascades. These profiles exhibit good consistency with the behaviors observed in other materials [10,12,36,43]. For comparison, the evolution of defects in pure Ni along with the simulation time is also displayed in Fig. 2(c), in agreement with the values of Béland et al. [43] used the same EAM potential. The number of defects increases rapidly at the beginning (*i.e.* ballistic phase), reaches its maximum value before 1 ps (*i.e.* thermal spike phase), and thereafter decreases slowly to a stable small value (*i.e.* annealing phase). This trend is independent of PKA energy and model system. With the enhancement of PKA energy, the peak value of defects and the time to peak increase accordingly in the thermal spike phase; the number of final surviving defects and the time to achieve system stability also increase in the annealing phase. Among them, the uneasy vacancies reach stability faster than uneasy interstitials: vacancies immobile before 10 ps, while interstitials almost stable before 15 ps. The cause for this can be that the diffusion barrier of interstitial is lower than that of vacancy in the bulk [17], which makes interstitials more susceptible to their surrounding lattice stress and cell temperature and then fluctuate frequently. These also suggest that the simulation time of 23 ps is enough for the cooling of thermal spike and the stabilization of defects and very beneficial to save computer time [44].

The stable defect production as a function of PKA energy is presented in Fig. 2(d). The number of surviving defects almost linearly increases with the increase of PKA energy either in NGNCs or in pure Ni, consistent with those of other works [32,37,43]. All these results are also well approximated by an NRT (Norgett–Robinson–Torrens) model [32,37,43].

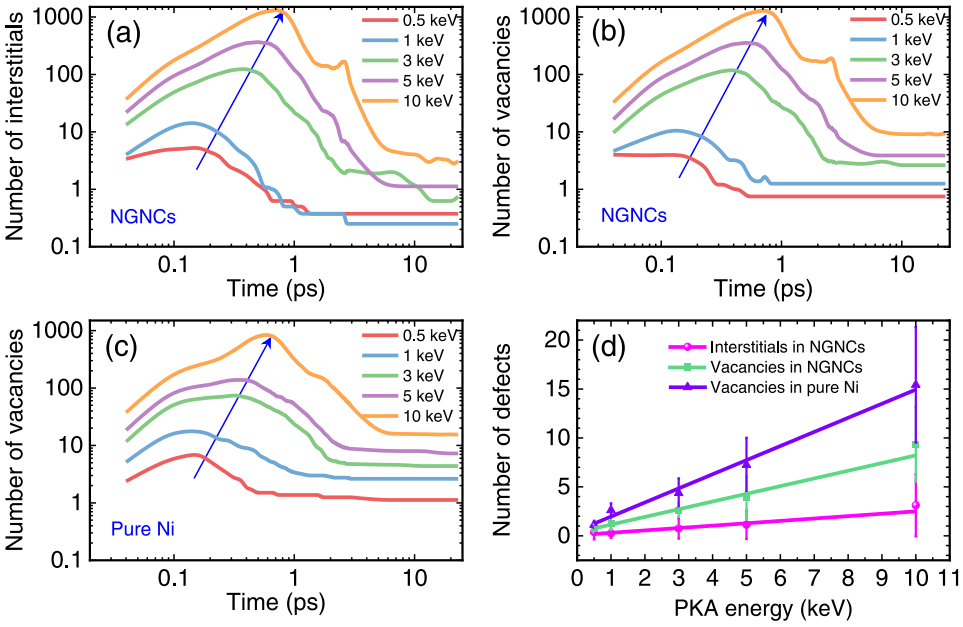


**Fig. 2.** Defect productions evoked by PKAs with 0.5, 1.0, 3.0, 5.0, and 10.0 keV. (a–c) Time evolution of point defects in NGNCs ((a) and (b)) and pure Ni (c), in which each line is an average of 10 runs. (d) Number of final surviving defects extracted from panels (a–c). Their linear fitting functions are: $y = 0.07 + 0.24x$, $R^2 = 0.89$ (pink line); $y = 0.36 + 0.78x$, $R^2 = 0.98$ (green line); $y = 0.52 + 1.44x$, $R^2 = 0.91$ (violet line). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

$$N_{def} = 0.4E_{PKA}/E_{d,} \quad (1)$$

where $N_{def}$ is the number of surviving defects, $E_{PKA}$ is the energy of a PKA, and $E_d$ is the displacement threshold energy of Ni atoms. An average threshold of 50 eV for the Bonny-based potentials is adopted herein [43]. It can be found that the defect production of MD simulations is significantly lower than that derived by the NRT model for the same PKA energy, because of not accounting for electronic stopping. For each PKA energy, the number of point defects in the bulk is substantially less than that in pure Ni. The difference between the two is more obvious with the increase of PKA energy. These suggest that NGIs can effectively facilitate the recombination and annihilation of irradiation defects. Moreover, the number of vacancies for each PKA energy is more than that of interstitials, once again confirming that NGIs preferentially capture interstitials over vacancies [17,31].

Due to the importance of Gr in forming NGIs, the morphology changes of Gr induced by displacement cascades with different energies need to be elaborated. Fig. 3 presents the surface morphologies of Gr at different moments during cascades. Either at the moment of thermal spike or the moment of thermal stability, the area of irradiation damage of Gr gradually increased with the increasing PKA energy, and the displacement degrees of C atoms along the z-axis were also intensified accordingly. Our molecular statics have shown that although the damage degree of Gr within the NGI gradually aggravates, the self-healing of irradiation defects in the bulk can be further enhanced by the NGI instead (*unpublished results*). As a result, the number of defects in Fig. 2 is also affected by the damaged Gr. The higher the PKA, the more outstanding the effect herein. Besides, the excessively displaced C atoms are not escaped from the Gr to enter the deep bulk region but absorbed on the Gr surface according to their z-coordinates. Compared with that of Gr at the moment of thermal spike, the damage of Gr at the moment of thermal stability realized a degree of self-repair. Especially, the damage of Gr completely disappeared and recovered to its original morphology at the moment of thermal stability after the bombardment of a PKA with 0.5 keV. The self-repair ability of Gr damage is also improved with the increase of PKA energy. The cause can be clarified as follows. First, displacement cascades not only lead to the damage of Gr but also generate instantaneous high temperature (up to thousands of degrees Kelvin far higher than the simulation temperature) in the vicinity of NGI through the effects of thermal spike [43,45,46]. Second, normally, it is difficult for the dangling C atoms on the Gr surface to return to their lattice positions due to the binding of C–C bonds [47]. However, the emergence of the instantaneous high temperature can trigger the dangling C atoms to move violently in the damaged region of Gr (*i.e.*, radiation-enhanced diffusion [48]) and then recombine continuously to realize the self-repair of Gr damage. This process can be called irradiation annealing [46]. Finally, with the increase of PKA energy, the instantaneous high temperature at the moment of thermal spike was elevated accordingly and more beneficial to enhance the irradiation annealing of Gr. Therefore, the damage of Gr does not destroy the interface structure obviously after the bombardment of energetic PKAs, and the role of NGI in healing radiation-induced defects is still able to play.

### 3.2. Elevated ambient temperature effects on displacement damage

This part focused on the influence of ambient temperature on the evolution of point defects. To avoid the synergistic effects of temperatures partially caused by thermal spike, only the behaviors of defects in the annealing phase were discussed. The stable defect production as a function of simulation temperature is presented in Fig. 4. The number of surviving defects (either interstitials or vacancies) in the bulk is less than that of pure Ni at each simulation temperature, indicating that NGIs can exhibit a good trapping ability to irradiation defects at all temperatures and promote the recombination and annihilation of point defects in the bulk. As temperature increases, the number of surviving defects in pure Ni shows an obvious declining trend, consistent with the results of previous studies [32]. This may be explained by the fact that the elevated temperature not only facilitates the migration of interstitials but also has enough energy to stimulate the migration of vacancies difficult to jump at low temperature, eventually promoting the recombination and annihilation of point defects. However, with the increasing temperature, the number of surviving defects in the bulk does not show the trend like that in pure Ni but fluctuates around a certain value. The fluctuation may come from multiple factors, including temperature and damaged NGI configuration. Furthermore, the number of interstitials is less than that of vacancies in the bulk at all temperatures, suggesting that the characteristic that NGIs preferentially trap interstitials is also independent of ambient temperature.

The surface morphologies of Gr and the damaged configurations of corresponding NGIs for different simulation temperatures at 23 ps are exhibited in Fig. 5. With the increasing temperature, the degree of

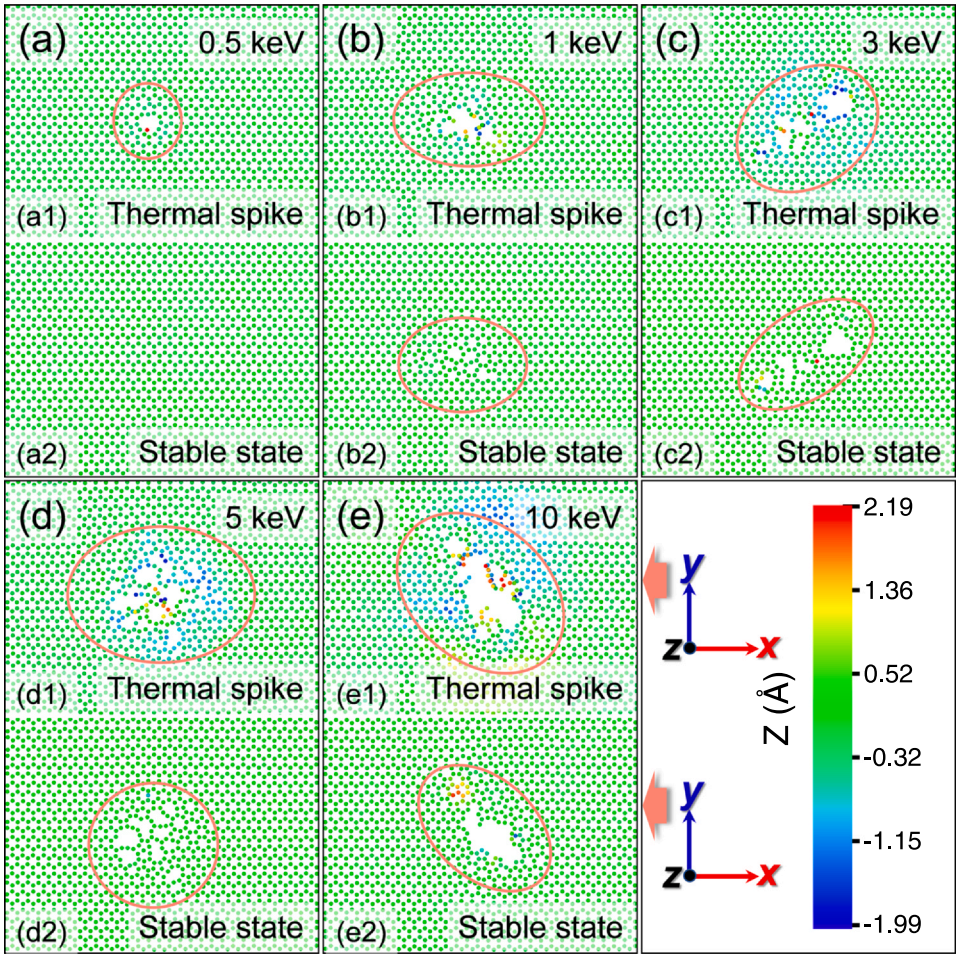


**Fig. 3.** Snapshots of the Gr of NGNCs captured at the moments of thermal spike and thermal stability, which are caused by a PKA with 0.5 (a), 1.0 (b), 3.0 (c), 5.0 (d), or 10.0 (e) keV. C atoms are colored according to their z-coordinates centering on the Gr plane. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

irradiation damage of Gr gradually aggravates. For example, the suspended C chains break continuously, and the damage area of Gr increases. However, the damage of Gr can be alleviated to some extent as the temperature exceeds 700 K, such as the decreasing damage area of Gr at 900 K relative to that at 700 K. By using electron beams to irradiate Gr, Song et al. [49] also found that the self-healing mechanisms of the radiation-induced damage of Gr will be activated when the ambient temperature is higher than 873 K. They attributed this behavior to the intrinsic property of Gr, that is, the irradiation damage of Gr can be repaired by the dangling C atoms on the Gr surface [49]. This self-healing process can be called ambient temperature annealing [50], different from the above irradiation annealing. Also, other studies have shown that Ni matrix can also promote the self-healing of Gr damage by a catalytic effect [51,52]. Therefore, it can be inferred that the damaged Gr of NGNCs may be self-healing at the ambient temperature below 873 K with the help of Ni matrix, such as the 700 K mentioned herein. The deterioration of Gr damage makes it easy for the Ni atoms above and below the Gr to penetrate the Ni layer on the other side of them, causing the miscibility of Ni atoms. The elevated temperature can further promote the diffusion and miscibility of Ni atoms. For example, although the damage degree of Gr is approximately equal at 500 K and 900 K, the miscibility of Ni atoms above and below the Gr is more serious at 900 K. Consequently, the special defect structure, with C and Ni defects simultaneously localized at the NGI, may strongly modify the NGI and thus, affect further evolution of irradiation defects near the NGI, one of the key factors for balancing the ambient temperature effects mentioned above on point defects in the bulk.

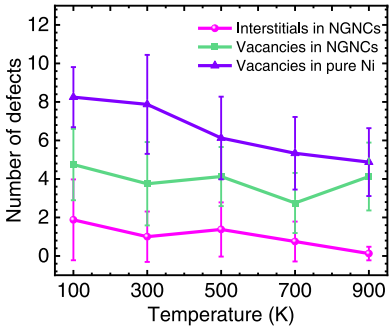


**Fig. 4.** Number of stable defects in NGNCs (or pure Ni) as a function of simulation temperature.

## 4. Conclusions

We have performed an investigation of energetic displacement cascades in NGNCs with different PKA energies and ambient temperatures using MD simulations. The following conclusions can be drawn from this work:

(a) With the improvement of PKA energy (in the interval 0.5–10 keV), the duration of thermal spike or annealing is prolonged, and more

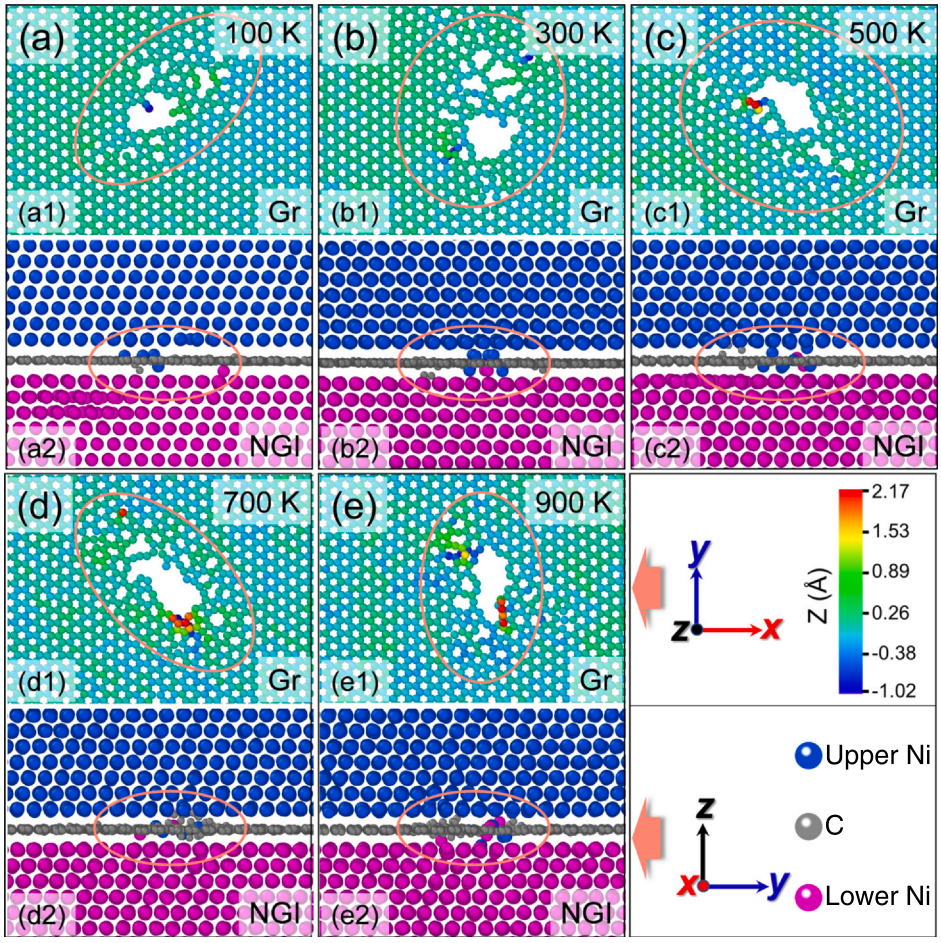


**Fig. 5.** Snapshots of the Gr morphologies and their corresponding NGI configurations for different simulation temperatures at 23 ps. (a) 100 K. (b) 300 K. (c) 500 K. (d) 700 K. (e) 900 K.

irradiation defects appear in the bulk. The deterioration of Gr damage becomes more obvious induced by the increasing cascade energy, but it can be self-healing to a certain extent through irradiation annealing.

(b) The number of surviving defects in the bulk is slightly affected by the change of ambient temperature (ranging from 100 K to 900 K), different from the situation of pure Ni. The Gr damage can be mitigated slightly due to the ambient temperature annealing as the simulation temperature exceeds 700 K.

(c) In all the above cases, NGIs show the ability to effectively facilitate the recombination and annihilation of irradiation defects and the preference to trap interstitials over vacancies. However, some issues about the influence of the damaged configurations of NGIs on their sink efficiency still need to be further addressed by future research. All these results can provide a reference for the assessment of the irradiation tolerance of NGNCs in the SCWRs.

## Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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## Appendix A. Supporting information

Supplementary data associated with this article can be found in the online version at doi:10.1016/j.supflu.2021.105162.

## References

[1] T. Schulenberg, L. Leung, Super-critical water-cooled reactors, in: I.L. Pioro (Ed.), Handbook of Generation IV Nuclear Reactors, Woodhead Publishing, Duxford, 2016, pp. 189–220.

[2] M.M. Rahman, J. Dongxu, N. Jahan, M. Salvatores, J. Zhao, Design concepts of supercritical water-cooled reactor (SCWR) and nuclear marine vessel: a review, Prog. Nucl. Energy 124 (2020) 103320, https://doi.org/10.1016/j.pnucene.2020.103320

[3] X. Guo, Y. Fan, W. Gao, R. Tang, K. Chen, Z. Shen, L. Zhang, Corrosion resistance of candidate cladding materials for supercritical water reactor, Ann. Nucl. Energy 127 (2019) 351–363, https://doi.org/10.1016/j.anucene.2018.12.007

[4] T.M. Osman, The nuclear renaissance: a challenge for the materials community, JOM 60 (2008) 10–13, https://doi.org/10.1007/s11837-008-0001-7

[5] K.L. Murty, I. Charit, Structural materials for Gen-IV nuclear reactors: challenges and opportunities, J. Nucl. Mater. 383 (2008) 189–195, https://doi.org/10.1016/j.jnucmat.2008.08.044

[6] I.J. Beyerlein, A. Caro, M.J. Demkowicz, N.A. Mara, A. Misra, B.P. Uberuaga, Radiation damage tolerant nanomaterials, Mater. Today 16 (2013) 443–449, https://doi.org/10.1016/j.mattod.2013.10.019

[7] X. Bai, B.P. Uberuaga, The influence of grain boundaries on radiation-induced point defect production in materials: a review of atomistic studies, JOM 65 (2013) 360–373, https://doi.org/10.1007/s11837-012-0544-5

[8] L. Tan, T.R. Allen, J.T. Busby, Grain boundary engineering for structure materials of nuclear reactors, J. Nucl. Mater. 441 (2013) 661–666, https://doi.org/10.1016/j.jnucmat.2013.03.050

[9] X. Zhang, K. Hattar, Y. Chen, L. Shao, J. Li, C. Sun, K. Yu, N. Li, M.L. Taheri, H. Wang, J. Wang, M. Nastasi, Radiation damage in nanostructured materials, Prog. Mater. Sci. 96 (2018) 217–321, https://doi.org/10.1016/j.pmatsci.2018.03.002

[10] B. Li, H. Li, S. Luo, Molecular dynamics simulations of displacement cascades in nanotwinned Cu, Comput. Mater. Sci. 152 (2018) 38–42, https://doi.org/10.1016/j.commatsci.2018.04.055

[11] N. Gao, D. Perez, G. Lu, Z. Wang, Molecular dynamics study of the interaction between nanoscale interstitial dislocation loops and grain boundaries in BCC iron, J. Nucl. Mater. 498 (2018) 378–386, https://doi.org/10.1016/j.jnucmat.2017.10.069
[12] X. Li, Y. Zhang, Y. Xu, X. Wu, X. Kong, X. Wang, Q. Fang, C. Liu, Interaction of radiation-induced defects with tungsten grain boundaries at across scales: a short review, Tungsten 2 (2020) 15–33, https://doi.org/10.1007/s42864-020-00039-5
[13] J. Chen, K. Dang, H.T. Vo, P. Hosemann, S.J. Fensin, Associating GB characteristics with its sink efficiency in absorbing Frank loops in Cu, Scr. Mater. 192 (2021) 61–66, https://doi.org/10.1016/j.scriptamat.2020.10.006
[14] Y. Kim, J. Baek, S. Kim, S. Kim, S. Ryu, S. Jeon, S.M. Han, Radiation resistant vanadium-graphene nanolayered composite, Sci. Rep. 6 (2016) 1–9, https://doi.org/10.1038/srep24785
[15] S. Si, W. Li, X. Zhao, M. Han, Y. Yue, W. Wu, S. Guo, X. Zhang, Z. Dai, X. Wang, X. Xiao, C. Jiang, Significant radiation tolerance and moderate reduction in thermal transport of a tungsten nanofilm by inserting monolayer graphene, Adv. Mater. 29 (2017) 1604623, https://doi.org/10.1002/adma.201604623
[16] T. Yang, L. Yang, H. Liu, H. Zhou, S. Peng, X. Zhou, F. Gao, X. Zu, Ab initio study of stability and migration of point defects in copper-graphene layered composite, J. Alloy. Compd. 692 (2017) 49–58, https://doi.org/10.1016/j.jallcom.2016.08.311
[17] H. Huang, X. Tang, F. Chen, F. Gao, Q. Peng, L. Ji, X. Sun, Self-healing mechanism of irradiation defects in nickel–graphene nanocomposite: an energetic and kinetic perspective, J. Alloy. Compd. 765 (2018) 253–263, https://doi.org/10.1016/j.jallcom.2018.06.162
[18] Y. Liu, Y. Zeng, Q. Guo, J. Zhang, Z. Li, D. Xiong, X. Li, D. Zhang, Bulk nanolaminated graphene (reduced graphene oxide)–aluminum composite tolerant of radiation damage, Acta Mater. 196 (2020) 17–29, https://doi.org/10.1016/j.actamat.2020.06.018
[19] D. Kuang, L. Xu, L. Liu, W. Hu, Y. Wu, Graphene–nickel composites, Appl. Surf. Sci. 273 (2013) 484–490, https://doi.org/10.1016/j.apsusc.2013.02.066
[20] S. Chang, A.K. Nair, M.J. Buehler, Geometry and temperature effects of the interfacial thermal conductance in copper–and nickel–graphene nanocomposites, J. Phys. Condens. Matter 24 (2012) 245301, https://doi.org/10.1088/0953-8984/24/24/245301
[21] H. Algul, M. Tokur, S. Ozcan, M. Uysal, T. Cetinkaya, H. Akbulut, A. Alp, The effect of graphene content and sliding speed on the wear mechanism of nickel–graphene nanocomposites, Appl. Surf. Sci. 359 (2015) 340–348, https://doi.org/10.1016/j.apsusc.2015.10.139
[22] J. Chen, J. Li, D. Xiong, Y. He, Y. Ji, Y. Qin, Preparation and tribological behavior of Ni-graphene composite coating under room temperature, Appl. Surf. Sci. 361 (2016) 49–56, https://doi.org/10.1016/j.apsusc.2015.11.094
[23] G. Yasin, M. Arif, M. Shakeel, Y. Dun, Y. Zuo, W.Q. Khan, Y. Tang, A. Khan, M. Nadeem, Exploring the nickel–graphene nanocomposite coatings for superior corrosion resistance: Manipulating the effect of deposition current density on its morphology, mechanical properties, and erosion–corrosion performance, Adv. Eng. Mater. 20 (2018) 1701166, https://doi.org/10.1002/adem.201701166
[24] Z. Chen, P. Wei, S. Zhang, B. Lu, L. Zhang, X. Yang, K. Huang, Y. Huang, X. Li, Q. Zhao, Graphene reinforced nickel-based superalloy composites fabricated by additive manufacturing, Mater. Sci. Eng. A 769 (2020) 138484, https://doi.org/10.1016/j.msea.2019.138484
[25] S. Bsat, B. Xiao, X. Huang, S. Penttilä, Oxidation behaviour of alloys 800H, 3033 and 304 in high-temperature supercritical water, Oxid. Met. 89 (2018) 151–163, https://doi.org/10.1007/s11085-017-9784-7
[26] S. Jin, X. He, T. Li, S. Ma, R. Tang, L. Guo, Microstructural evolution in nickel alloy C-276 after Ar-ion irradiation at elevated temperature, Mater. Charact. 72 (2012) 8–14, https://doi.org/10.1016/j.matchar.2012.06.010
[27] S. Teysseyre, Z. Jiao, E. West, G.S. Was, Effect of irradiation on stress corrosion cracking in supercritical water, J. Nucl. Mater. 371 (2007) 107–117, https://doi.org/10.1016/j.jnucmat.2007.05.008
[28] K.I. Fukumoto, M. Nishimura, H. Matsui, M. Yamazaki, Mechanical properties and microstructure in neutron-irradiated nickel-based alloys and stainless steels for supercritical water-cooled-reactor fuel cladding, J. Nucl. Sci. Technol. 57 (2020) 114–120, https://doi.org/10.1080/00223131.2019.1660730
[29] H. Huang, X. Tang, F. Chen, J. Liu, X. Sun, L. Ji, Radiation tolerance of nickel–graphene nanocomposite with disordered graphene, J. Nucl. Mater. 510 (2018) 1–9, https://doi.org/10.1016/j.jnucmat.2018.07.051
[30] G. Ge, F. Chen, X. Tang, H. Huang, X. Sun, L. Ji, Phase-field modeling of helium bubble evolution in nickel-graphene nanocomposite, J. Appl. Phys. 125 (2019) 215304, https://doi.org/10.1063/1.5084238
[31] H. Huang, X. Tang, F. Gao, F. Chen, G. Ge, Y. Yan, Q. Peng, Release of helium-related clusters through a nickel–graphene interface: an atomistic study, Appl. Surf. Sci. 487 (2019) 218–227, https://doi.org/10.1016/j.apsusc.2019.05.085
[32] D.J. Bacon, F. Gao, Y.N. Osetsky, The primary damage state in fcc, bcc and hcp metals as seen in molecular dynamics simulations, J. Nucl. Mater. 276 (2000) 1–12, https://doi.org/10.1016/S0022-3115(99)00165-8
[33] K. Nordlund, F. Djurabekova, Multiscale modelling of irradiation in nanostructures, J. Comput. Electron. 13 (2014) 122–141, https://doi.org/10.1007/s10825-013-0542-z
[34] E. Zarkadoula, G. Samolyuk, W.J. Weber, Effects of electron–phonon coupling on damage accumulation in molecular dynamics simulations of irradiated nickel, Mater. Res. Lett. 7 (2019) 490–495, https://doi.org/10.1080/21663831.2019.1659435
[35] C. Maxwell, J. Pencer, E. Torres, Atomistic simulation study of clustering and evolution of irradiation-induced defects in zirconium, J. Nucl. Mater. 531 (2020) 151979, https://doi.org/10.1016/j.jnucmat.2019.151979
[36] W. Zhou, J. Tian, Q. Feng, J. Zheng, X. Liu, J. Xue, D. Qian, S. Peng, Molecular dynamics simulations of high-energy displacement cascades in hcp-Zr, J. Nucl. Mater. 508 (2018) 540–545, https://doi.org/10.1016/j.jnucmat.2018.06.002
[37] N.P. Lazarev, A.S. Bakai, Atomistic simulation of primary damages in Fe, Ni and Zr, J. Supercrit. Fluids 82 (2013) 22–26, https://doi.org/10.1016/j.supflu.2013.06.002
[38] S.J. Stuart, A.B. Tutein, J.A. Harrison, A reactive potential for hydrocarbons with intermolecular interactions, J. Chem. Phys. 112 (2000) 6472–6486, https://doi.org/10.1063/1.481208
[39] G. Bonny, N. Castin, D. Terentyev, Interatomic potential for studying ageing under irradiation in stainless steels: the FeNiCr model alloy, Model. Simul. Mater. Sci. Eng. 21 (2013) 085004, https://doi.org/10.1088/0965-0393/21/8/085004
[40] S.P. Huang, D.S. Mainardi, P.B. Balbuena, Structure and dynamics of graphite-supported bimetallic nanoclusters, Surf. Sci. 545 (2003) 163–179, https://doi.org/10.1016/j.susc.2003.08.050
[41] S. Plimpton, Fast parallel algorithms for short-range molecular dynamics, J. Comput. Phys. 117 (1995) 1–19, https://doi.org/10.1006/jcph.1995.1039
[42] A. Stukowski, Visualization and analysis of atomistic simulation data with OVITO – the Open Visualization Tool, Model. Simul. Mater. Sci. Eng. 18 (2009) 015012, https://doi.org/10.1088/0965-0393/18/1/015012
[43] L.K. Béland, C. Lu, Y.N. Osetskiy, G.D. Samolyuk, A. Caro, L. Wang, R.E. Stoller, Features of primary damage by high energy displacement cascades in concentrated Ni-based alloys, J. Appl. Phys. 119 (2016) 085901, https://doi.org/10.1063/1.4942533
[44] Y. Dai, L. Ao, Q. Sun, L. Yang, J. Nie, S. Peng, X. Long, X. Zhou, X. Zu, L. Liu, X. Sun, D. Terentyev, F. Gao, Nucleation of Cr precipitates in Fe–Cr alloy under irradiation, Comput. Mater. Sci. 101 (2015) 293–300, https://doi.org/10.1016/j.commatsci.2015.01.015
[45] T.D. De La Rubia, R.S. Averback, H. Hsieh, R. Benedek, Molecular dynamics simulation of displacement cascades in Cu and Ni: thermal spike behavior, J. Mater. Res. 4 (1989) 579–586, https://doi.org/10.1557/JMR.1989.0579
[46] Y. Lin, T. Yang, L. Lang, C. Shan, H. Deng, W. Hu, F. Gao, Enhanced radiation tolerance of the Ni-Co-Cr-Fe high-entropy alloy as revealed from primary damage, Acta Mater. 196 (2020) 133–143, https://doi.org/10.1016/j.actamat.2020.06.027
[47] P. Vinchon, X. Glad, G.R. Bigras, R. Martel, L. Stafford, Preferential self-healing at grain boundaries in plasma-treated graphene, Nat. Mater. 20 (2021) 49–54, https://doi.org/10.1038/s41563-020-0738-0
[48] G.S. Was, Radiation-enhanced diffusion and defect reaction rate theory, in: G.S. Was (Ed.), Fundamentals of Radiation Materials Science, Springer, New York, 2017, pp. 207–252.
[49] B. Song, G.F. Schneider, Q. Xu, G. Pandraud, C. Dekker, H. Zandbergen, Atomic-scale electron-beam sculpting of near-defect-free graphene nanostructures, Nano Lett. 11 (2011) 2247–2250, https://doi.org/10.1021/nl200369r
[50] J. Zhu, D. Shi, A possible self-healing mechanism in damaged graphene by heat treatment, Comput. Mater. Sci. 68 (2013) 391–395, https://doi.org/10.1016/j.commatsci.2012.10.041
[51] S. Karoui, H. Amara, C. Bichara, F. Ducastelle, Nickel-assisted healing of defective graphene, ACS Nano 4 (2010) 6114–6120, https://doi.org/10.1021/nn101822s
[52] P. Jacobson, B. Stöger, A. Garhofer, G.S. Parkinson, M. Schmid, R. Caudillo, F. Mittendorfer, J. Redinger, U. Diebold, Disorder and defect healing in graphene on Ni (111), J. Phys. Chem. Lett. 3 (2012) 136–139, https://doi.org/10.1021/jz2015007