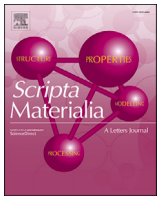
Scripta Materialia 242 (2024) 115902

Contents lists available at ScienceDirect

Scripta Materialia

journal homepage: www.journals.elsevier.com/scripta-materialia



Explaining the effect of in-plane strain on thermal degradation kinetics of Cu/W nano-multilayers

Javier F. Troncoso [a,1], Giacomo Lorenzin [b,1], Claudia Cancellieri [b,*], Vladyslav Turlo [a,c,*]

[a] Laboratory for Advanced Materials Processing, Empa - Swiss Federal Laboratories for Materials Science and Technology, Thun, Switzerland
[b] Laboratory for Joining Technologies and Corrosion, Empa - Swiss Federal Laboratories for Materials Science and Technology, Duebendorf, Switzerland
[c] National Centre for Computational Design and Discovery of Novel Materials MARVEL, Empa, Thun, Switzerland

ARTICLE INFO

Dataset link: https://doi.org/10.24435/materialscloud:ah-f4

Keywords:
Nano-multilayers
Degradation kinetics
Cu/W
In-plane strain
Vacancy-driven diffusion
Ab initio calculations

ABSTRACT

Thermal annealing experiments evidence opposite effect on the degradation kinetics of Cu/W nano-multilayers from compressive to tensile in-plane strain. Besides higher activation energy, nano-multilayers with tensile strains degrade to nanocomposites faster than those with compressive strains. By assuming a vacancy-driven diffusion mechanism of degradation, we applied *ab initio* calculations to quantify different contributions to the corresponding diffusion coefficients in relation to in-plane strain. The average vacancy formation energy increases as the strain changes from compressive to tensile, which explains the higher experimental activation energy. The bulk in-plane and out-of-plane vacancy migration energies and corresponding diffusion prefactors highlight that enhanced transformation rate under tension can be explained by the segregation of non-equilibrium W vacancies to Cu/W interfaces. These theoretical insights are grounded in and serve to interpret the experimental observations, offering a coherent understanding of the strain-dependent thermal degradation kinetics.

The immiscible copper/tungsten (Cu/W) system has attracted attention in the scientific community in the last years because of the combination of the good electrical and thermal properties of Cu with the excellent mechanical properties of W [1–4]. This finds multiple applications as heat sinks in electronic devices, nuclear fusion components, or packaging components [3,5]. Due to the complete immiscibility between Cu and W, interface effects play an important role in these structures and the resulting mechanical, optical, magnetic, thermal, and electronic properties of the system can be tailored through microstructural and interfacial design [4]. The interface structure in immiscible fcc/bcc metallic systems is complex and still not well understood [6,7], but it plays a decisive role in the properties and stability of Cu/W nano-multilayers (NMLs) [2]. In the Cu/W system, the origin and structure of the interfaces have been controversial for many years in the literature [8–11,7]. In NMLs, interfaces account for a significant volume fraction of the material [5], so their study is crucial to understand the properties of the NMLs. The design of Cu/W NMLs combining nanometer-size layers amplifies the characteristics of the heterogeneous interfaces and produces structures with unique properties, different from those of the corresponding bulk materials. The high excess energy associated with the presence of interfaces affects the thermal properties and the thermal stability of NMLs, which are highly technological relevant. The presence of large interface stresses [4] affects the chemical properties of the interfaces and promotes the diffusion of Cu atoms [12]. At high temperatures (700 °C), the microstructure stability can be strongly compromised by the thermodynamic driving force to minimize the energies of internal boundaries, such as high-energetical grain boundaries (GB). Upon annealing, grooving of GB is a possible way to minimize the internal energy. This brings to the transformation of the NML into a nanocomposite (NC) [13,14]. Prior to NML degradation, i.e., in the temperature range of 400 – 600 °C, the Cu/W NML system first releases the accommodated residual stresses in the Cu and W nanolayers (while maintaining the multilayer structure) [15]. The activation energy of the degradation process into NC has been found experimentally to be rate limited by W mobility along GB and interphase boundaries [14]. The internal stress and interface defects have an important role in determining the activation energy of NML degradation. For example, in-plane compressive residual stress and defects induced by ion beam deposition result in low thermal stability. Moreover, the mechanism driving to the

* Corresponding authors.
E-mail addresses: Claudia.Cancellieri@empa.ch (C. Cancellieri), Vladyslav.Turlo@empa.ch (V. Turlo).
[1] Equal contribution.

https://doi.org/10.1016/j.scriptamat.2023.115902
Received 31 August 2023; Received in revised form 2 November 2023; Accepted 24 November 2023
Available online 30 November 2023

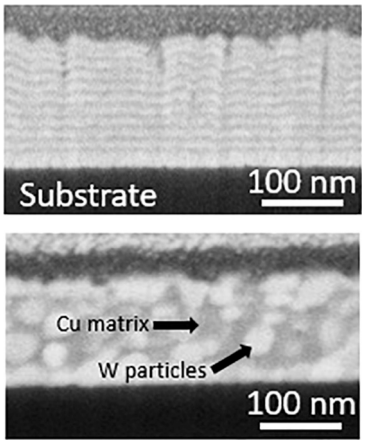


Fig. 1. SEM cross sections of a NML before (top) and after (bottom) NC transformation.

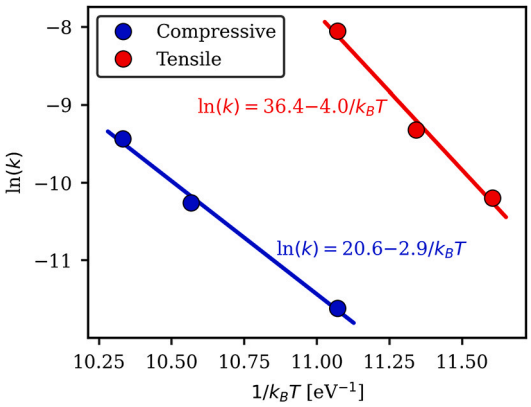


Fig. 2. Arrhenius plot for the activation energy of NC transformation for compressive and tensile NMLs. (For interpretation of the colors in the figure(s), the reader is referred to the web version of this article.)

complete degradation of the layered structure was identified to be the thermally activated self-interstitial and vacancy diffusion [16].

The different residual and interface stress states in NMLs can be achieved by tuning structural parameters, e.g., Cu and W layer thicknesses and substrate material, or process parameters, such as chamber gas pressure, magnetron power, temperature, etc. All these parameters allow for creating NMLs with different as-deposited in-plane stress states and microstructure that can influence both thermal stability and NML-to-NC transformation rates [17,18]. The internal stress and the associated microstructure [19] are found to influence most the observed NML to NC degradation. In this work, we investigated the effect of the in-plane stress on the activation energy and degradation kinetics of Cu/W NML into NC. The internal stress tuning was achieved by changing the working pressure during the sputtering growth while all the other parameters (e.g., thickness, substrate and temperature) were kept constant. Key elements for understanding the dynamics of nanoscale diffusion including vacancy-driven diffusion mechanism of degradation are computed by *ab initio* calculations.

An example of NML-to-NC transformation under annealing is shown in Fig. 1 where after treatment at 800 °C in vacuum for 100 min, the periodic NML structure is destroyed. To understand the effect of in-plane stress on the degradation of Cu/W NMLs, we performed a series of *in situ* high-temperature XRD experiments with NMLs prepared under two different processing conditions, leading to opposite in-plane stress states, i.e., tensile and compressive [17]. The details of the deposition, annealing experiments and the in-plane stress values are provided in the Supplementary Materials, and the final results are summarized in Fig. 2. Each point in this graph is derived from the decay rate, k, of the XRD satellite peak corresponding to Cu/W multilayer structure (same procedure used in [14]), in relation to the initial compressive (blue) and tensile (red) residual stresses in NMLs. The presence of modulated XRD intensity oscillations, giving rise to the so-called satellite peaks, is typical for a periodic nanolayered structure along the z axis. When a NML transforms upon annealing into a NC, satellite peaks disappear leaving only single peaks of the component materials: Cu(111) and W(110). By following the decay of the satellite integrated intensity with time at high temperature, we can derive the NML-to-NC transformation rate, k, for different isothermal treatments [14]. The details of this procedure are provided in Supplementary Materials. Fig. 2 represents the Arrhenius plot in relation to the annealing temperature, allowing us to extract the corresponding activation energy for the NML degradation process. Interestingly, the activation energy for samples with tensile in-plane stresses is more than 1 eV higher than for samples with compressive stresses, and still, the transformation rate to NC is substantially higher for samples with tensile stress.

To make a first crack at this puzzle, we will further interpret the experimental observations assuming interface vacancy-driven NML degradation kinetics, as the atomic shuffling diffusion mechanism is highly unlikely at the experimental temperatures that are well below the melting point of Cu and W. Generally, vacancies play an essential role in the kinetic, thermodynamic, electrical, optical, and mechanical properties of solids [20]. In particular, interfacial vacancies can strongly affect diffusion at the interfaces, changing their local atomic density, structure, and energy [21–23]. At the same time, heterogeneous interfaces and grain boundaries can act both as vacancy sources and sinks depending on the vacancy saturation levels in the bulk phases [23].

Ab initio calculations were successfully applied in the past to characterize vacancy-driven atomic transport in the metastable Cu/W composites [24,25]. Thus, we use density functional theory (DFT) calculations in the CP2K code [26] to investigate the formation and migration of vacancies at different in-plane strain states in bulk Cu and W, as well as their interfaces. Our DFT calculations were based on the Gaussian and plane wave (GPW) method [27] with the plane wave cutoff at 500 Ry and the Goedecker–Teter–Hutter pseudopotential [28]. The Cu(111)/W(110) interfaces are studied in this work as they have been observed with the highest frequency in experiments [29,15]. The simulation box containing 245 Cu atoms and 200 W atoms under periodic boundary conditions was generated with the CellMatch code [30] to minimize the residual in-plane mismatch between Cu and W blocks to 0.7%. Due to the large (~ 23%) lattice mismatch between Cu and W [25], no misfit dislocations are expected to form at the fully incoherent Cu/W interfaces. Fig. 3a shows the reference state of the bilayer after DFT supercell relaxation to zero stress in all directions, balancing residual in-plane stress in each layer with the interface stress. Such a bilayer system is further considered as the 0 strain reference sample, even though in-plane strain in adjunct Cu and W layers are non-zero due to an initial mismatch of 0.7% mostly isolated in the Cu layer. We studied the effect of in-plain strain equally applied in all directions parallel to the interface on the vacancy formation energy at the interfacial Cu and W planes. The calculation procedure is explained in detail in Supplementary Materials.

Fig. 3b shows the vacancy formation energy distribution in the interfacial Cu/W planes at zero applied strain. The energy of vacancy formation varies randomly depending on the lattice site from which the atom is removed, due to the complete incoherence of the interface, i.e., the absence of misfit dislocations and stacking faults. Because of the extreme difference in Cu and W vacancy formation energies in some areas of the interface, some W vacancy sites get occupied by neighboring Cu atoms, indicating barrierless migration of W vacancy to the Cu plane (see Supplementary Video S1). Such a move would introduce some degree of intermixing at the interface, which seems to be more energetically favorable than keeping such vacancies at the W plane. We provide Supplementary Videos to show the movement of atoms during W vacancy relaxation to illustrate these observations. However, the bar-

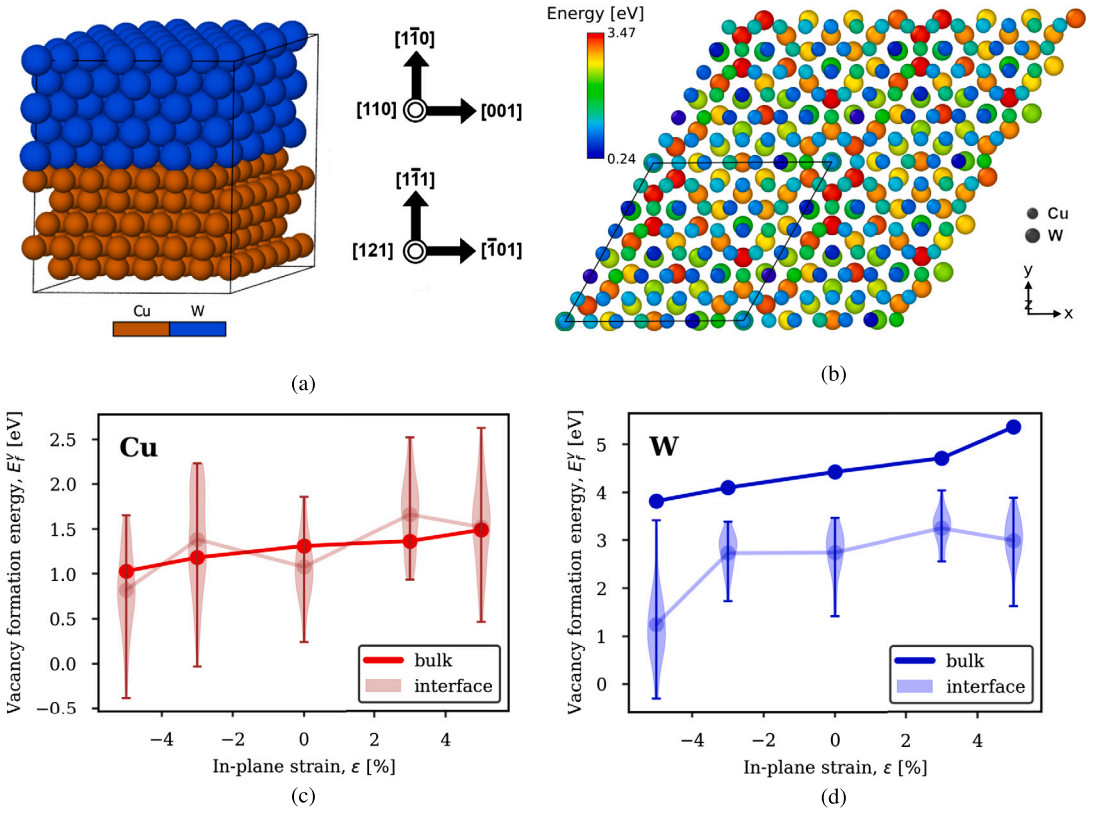


Fig. 3. (a) Simulation box used in the study of interface properties in Cu(111)/W(110) NMLs. Periodic boundary conditions were applied in all directions. (b) Vacancy formation energies of interfacial atoms in the Cu/W bilayer shown in (a) replicated 2×2 times in the direction perpendicular to the interface, under no applied in-plane strain ($\epsilon = 0\%$). (c) Vacancy formation energies of interfacial Cu atoms in the Cu/W bilayer shown in (a) under different applied in-plane strains (ϵ), compared with bulk values. (d) Distribution of vacancy formation energies to create a single vacancy at the interfacial W plane, compared with the value in bulk, at different in-plane strains.

rierless migration of the W vacancy to the Cu side is an exception rather than the rule. The more common relaxation mechanism is the nearest Cu atom moving towards the vacancy and stopping near halfway, essentially delocalizing the vacancy between Cu and W planes and distorting the positions of the nearest neighbors at the interface. This can be interpreted as a possible mechanism of Cu/W interface disordering.

Moving forward to the effect of the in-plane strain, we computed the distributions of vacancy formation energies at the interfacial Cu and W planes for -5% and -3% compressive strains, as well as +3% and +5% tensile strains, and added the corresponding figures similar to Fig. 3b as the Supplementary Fig. S3. At all strains including zero strain, the interfacial vacancy formation energies are characterized by wide distributions and scattering in values rather randomly over the interface area. To characterize such distributions in statistical terms, we also computed mean, median, minimum, and maximum values separately for Cu and W, and reported them in Supplementary Table 1. Figs. 3c and 3d demonstrate complete distributions together with the mean values in each distribution, as well as the corresponding bulk values, i.e., the vacancy formation energies in pure Cu and W at the same level of in-plane strain. For all strains tested, the mean interfacial Cu values are similar to those of the bulk Cu, whereas the mean and generally all interfacial W values are substantially lower than the corresponding bulk W values. Thus, we can expect interface segregation of non-equilibrium W vacancies to and across the interface at any in-plane strain.

In common for both Cu and W, the vacancy formation energy generally increases with increasing in-plane strain, meaning that vacancy formation is more favorable under compression, both in the bulk and at the interface. Furthermore, under extreme compressive stresses, vacancy formation at certain interfacial sites is energetically favorable even at 0 K, as indicated by their negative energy values. The formation of vacancies under compressive stress is promoted because the resulting free volume added to the system relaxes its excess strain energy. As the vacancy formation energy is part of the activation energy for vacancy-driven diffusion, this trend explains well our experimental observations, i.e., the increasing activation energy while moving from compressive to tensile stress in Fig. 2.

To understand why the transformation rate to nanocomposites is orders of magnitude higher for tensile stresses than for compressive stresses besides the lower activation energy for the latter, we have to consider the mobility of non-equilibrium vacancies created in the multilayers during the deposition process. The bulk vacancy diffusion coefficient is proportional to:

$$D \propto D_0 \cdot \exp\left(-\frac{E_v^m}{k_B T}\right) \equiv K, \tag{1}$$

where E_v^m is migration energy, D_0 is the diffusion prefactor, k_B is Boltzmann constant, and T is temperature in the system. Here, K can characterize the directional mobility of supersaturated vacancies in the system. When a vacancy is introduced into the bulk Cu and W DFT supercells, we introduce substantially high vacancy concentrations of around 0.7% for Cu and 0.6% for W. By calculating the corresponding energies and prefactors of bulk vacancy migration in the direction perpendicular to the straining direction, we can characterize segregation kinetics of such supersaturated vacancies towards Cu/W interfaces in the Cu/W nano-multilayers. The computational details for such calculations are provided in Supplementary Materials, and the final results are provided in Table 1 with the K factor predicted for 1050 K corresponding to the overlapping temperature in Fig. 2 i.e., the highest temperature for the tensile samples and the lowest temperature for the compressive samples (~ 775°C). As first, we can notice is how little all

Table 1
Computed vacancy migration energies E_v^m, diffusion prefactors D_0, and directional mobility factor K in bulk Cu and W when the vacancy moves perpendicular to the applied in-plane strain ϵ.

ϵ [%]	E_v^m [eV]		D_0 [m^2/s]		K (1050 K) [m^2/s]	
	Cu	W	Cu	W	Cu	W
-3	0.82	2.39	$1.66 \cdot 10^{-5}$	$1.02 \cdot 10^{-5}$	$1.94 \cdot 10^{-9}$	$3.44 \cdot 10^{-17}$
0	0.82	2.08	$1.32 \cdot 10^{-5}$	$1.46 \cdot 10^{-5}$	$1.53 \cdot 10^{-9}$	$1.52 \cdot 10^{-15}$
+3	0.73	1.07	$1.37 \cdot 10^{-5}$	$1.38 \cdot 10^{-5}$	$4.29 \cdot 10^{-9}$	$1.01 \cdot 10^{-10}$

quantities change for Cu so that even extreme variation of strain from -3 to 3% does not change the order of magnitude of K, which reinforces the idea that Cu diffusion does not affect the nano-multilayer degradation process in any way. Contrary to that, K factor for W is varying by 7 orders of magnitude in this strain range with more variation coming under tension. As the corresponding prefactor stays in the same order of magnitude, such variation in K is attributed to substantial decrease in vacancy migration energy under tension. Experimental results in Fig. 2 demonstrate over 4 orders of magnitude increase in degradation rate, which can be explained by more modest strain variation in range of -1 to 1%.

Thus, we can conclude that the Cu/W nano-multilayer degradation process is controlled by two processes acting together: supersaturated W vacancy segregation to the Cu/W interfaces and W interfacial diffusion. The difference in microstructure between compressive and tensile stress NMLs is reported also to affect the NML to NC transition [18] and thus final degradation rate and activation energy. Further processes of grain boundary wetting and grooving must be investigated by means of large-scale atomistic simulations and phenomenological modeling to gain complete understanding of the process, and is a matter of follow-up work. Our work increases the piling stack of evidence suggesting that in NMLs made of two metals with large differences in melting points, the degradation process is controlled by the diffusion of more refractory metal [31]. All these insights on the degradation kinetics of metallic NMLs in relation with the internal stress are highly relevant for controlling and understanding the microstructure modification in multilayers aiming to tailor nanocomposite properties for specific applications, adding one more control dimension, i.e., in-plane strain. Other control variables are the annealing temperature, the concentration of non-equilibrium W vacancies, and W layer thickness defining the effective diffusion length of such vacancies to the Cu/W interfaces.

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.

Data availability

The data used in the present work is available here: https://doi.org/10.24435/materialscloud:ah-f4.

Acknowledgements

We thank Carlo Pignedoli for his help with the CP2K code, and Olivier Politano, Florence Baras, Helena Zapolsky, Lars Jeurgens, and Aleksandr Druzhinin for fruitful discussions. This research was supported by the NCCR MARVEL, a National Centre of Competence in Research, funded by the Swiss National Science Foundation (grant number 205602). Also, we thank CSCS for providing computing resources under project s1130. G.L. acknowledges the Swiss National Science Foundation (SNSF) under Project No. 200021_192224 for financially supporting this research. V.T. thanks the Bern Economic Development Agency for financial support.

Appendix A. Supplementary material

Supplementary material related to this article can be found online at https://doi.org/10.1016/j.scriptamat.2023.115902.

References

[1] W.M. Daoush, J. Yao, M. Shamma, K. Morsi, Ultra-rapid processing of high-hardness tungsten-copper nanocomposites, Scr. Mater. 113 (2016) 246–249, https://doi.org/10.1016/j.scriptamat.2015.11.012.
[2] G.C. Ma, J.L. Fan, H.R. Gong, Mechanical behavior of Cu-W interface systems upon tensile loading from molecular dynamics simulations, Comput. Mater. Sci. 152 (2018) 165–168, https://doi.org/10.1016/j.commatsci.2018.05.030.
[3] W. Wei, L. Chen, H.R. Gong, J.L. Fan, Strain-stress relationship and dislocation evolution of W-Cu bilayers from a constructed n-body W-Cu potential, J. Phys. Condens. Matter 31 (2019), https://doi.org/10.1088/1361-648X/ab1a8a.
[4] A.V. Druzhinin, G. Lorenzin, D. Ariosa, S. Siol, B.B. Straumal, J. Janczak-Rusch, L.P. Jeurgens, C. Cancellieri, The effect of the graded bilayer design on the strain depth profiles and microstructure of Cu/W nano-multilayers, Mater. Des. 209 (2021), https://doi.org/10.1016/j.matdes.2021.110002.
[5] A. Sáenz-Trevizo, A.M. Hodge, Nanomaterials by design: a review of nanoscale metallic multilayers, Nanotechnology 31 (2020), https://doi.org/10.1088/1361-6528/ab803f.
[6] G. Gładyszewski, J. Pacaud, P. Goudeau, C. Jaouen, A. Naudon, J. Grilhé, Interface of the CuW multilayers, Vacuum 45 (2–3) (1994) 285–287, https://doi.org/10.1016/0042-207X(94)90190-2.
[7] C.P. Liang, J.L. Fan, H.R. Gong, X. Liao, X. Zhu, S. Peng, Interface structure and work function of W-Cu interfaces, Appl. Phys. Lett. 103 (2013), https://doi.org/10.1063/1.4833249.
[8] N.J. Taylor, A LEED study of the epitaxial growth of copper on the (110) surface of tungsten, Surf. Sci. 4 (2) (1966) 161–194, https://doi.org/10.1016/0039-6028(66)90075-6.
[9] E. Bauer, H. Poppa, G. Todd, F. Bonczek, Adsorption and condensation of Cu on W single-crystal surfaces, J. Appl. Phys. 45 (12) (1974) 5164–5175, https://doi.org/10.1063/1.1663211.
[10] A. Cetronio, J.P. Jones, E.W. Roberts, A study of copper adsorption on (100) tungsten by high field microscopy, Surf. Sci. 52 (3) (1975) 473–488, https://doi.org/10.1016/0039-6028(75)90082-5.
[11] K. Reshöft, C. Jensen, U. Köhler, Atomistics of the epitaxial growth of Cu on W(110), Surf. Sci. 421 (3) (1999) 320–336, https://doi.org/10.1016/S0039-6028(98)00859-0.
[12] A.V. Druzhinin, B. Rheingans, S. Siol, B.B. Straumal, J. Janczak-Rusch, L.P. Jeurgens, C. Cancellieri, Effect of internal stress on short-circuit diffusion in thin films and nanolaminates: application to Cu/W nano-multilayers, Appl. Surf. Sci. 508 (2020), https://doi.org/10.1016/j.apsusc.2020.145254.
[13] H. Li, Z.-C. Xing, B. jin Li, X.-S. Liu, B. Lehmert, M. Matthias, Z. xin Li, W. Tillmann, Microstructural evolution of Cu/W nano-multilayers filler metal during thermal treatment, Vacuum 200 (2022) 111007, https://doi.org/10.1016/j.vacuum.2022.111007.
[14] F. Moszner, C. Cancellieri, M. Chiodi, S. Yoon, D. Ariosa, J. Janczak-Rusch, L.P. Jeurgens, Thermal stability of Cu/W nano-multilayers, Acta Mater. 107 (2016) 345–353, https://doi.org/10.1016/j.actamat.2016.02.003.
[15] C. Cancellieri, F. Moszner, M. Chiodi, S. Yoon, J. Janczak-Rusch, L.P.H. Jeurgens, The effect of thermal treatment on the stress state and evolving microstructure of Cu/W nano-multilayers, J. Appl. Phys. 120 (19) (2016) 195107, https://doi.org/10.1063/1.4967992.
[16] L. Romano-Brandt, E. Salvati, D. Wermeille, C. Papadaki, E. Le Bourhis, A.M. Korsunsky, Stress-assisted thermal diffusion barrier breakdown in ion beam deposited Cu/W nano-multilayers on Si substrate observed by in situ GISAXS and transmission EDX, ACS Appl. Mater. Interfaces 13 (5) (2021) 6795–6804, https://doi.org/10.1021/acsami.0c19173.

[17] G. Lorenzin, L.P.H. Jeurgens, C. Cancellieri, Stress tuning in sputter-grown Cu and W films for Cu/W nanomultilayer design, J. Appl. Phys. 131 (22) (2022) 225304, https://doi.org/10.1063/5.0088203.
[18] G. Lorenzin, M.S.B. Hoque, D. Ariosa, L.P. Jeurgens, E.R. Hoglund, J.A. Tomko, P.E. Hopkins, C. Cancellieri, Tensile and compressive stresses in Cu/W multilayers: correlation with microstructure, thermal stability, and thermal conductivity, Acta Mater. 240 (2022) 118315, https://doi.org/10.1016/j.actamat.2022.118315.
[19] C. Cancellieri, G. Lorenzin, L.P.H. Jeurgens, Microstructure-property control in functional materials by multilayer design, Chimia 76 (3) (2022) 223, https://doi.org/10.2533/chimia.2022.223.
[20] G. Lu, N. Kioussis, Interaction of vacancies with a grain boundary in aluminum: a first-principles study, Phys. Rev. B, Condens. Matter Mater. Phys. 64 (2) (2001) 1–7, https://doi.org/10.1103/PhysRevB.64.024101.
[21] M. Mazalová, M. Všianská, J. Pavlů, M. Šob, The effect of vacancies on grain boundary segregation in ferromagnetic fcc Ni, Nanomaterials 10 (2020), https://doi.org/10.3390/nano10040691.
[22] D.S. Sholl, R.T. Skodje, Diffusion of clusters of atoms and vacancies on surfaces and the dynamics of diffusion-driven coarsening, Phys. Rev. Lett. 75 (17) (1995) 3158–3161, https://doi.org/10.1103/PhysRevLett.75.3158.
[23] G.B. McFadden, W.J. Boettinger, Y. Mishin, Effect of vacancy creation and annihilation on grain boundary motion, Acta Mater. 185 (2020) 66–79, https://doi.org/10.1016/j.actamat.2019.11.044.
[24] C. González, R. Iglesias, Energetic analysis of He and monovacancies in Cu/W metallic interfaces, Mater. Des. 91 (2016) 171–179, https://doi.org/10.1016/j.matdes.2015.11.097.
[25] R. Bodlos, V. Fotopoulos, J. Spitaler, A.L. Shluger, L. Romaner, Energies and structures of Cu/Nb and Cu/W interfaces from density functional theory and semi-empirical calculations, Materialia 21 (2022) 101362, https://doi.org/10.1016/j.mtla.2022.101362.
[26] T.D. Kühne, M. Iannuzzi, M. Del Ben, V.V. Rybkin, P. Seewald, F. Stein, T. Laino, R.Z. Khaliullin, O. Schütt, F. Schiffmann, D. Golze, J. Wilhelm, S. Chulkov, M.H. Bani-Hashemian, V. Weber, U. Borštnik, M. Taillefumier, A.S. Jakobovits, A. Lazzaro, H. Pabst, T. Müller, R. Schade, M. Guidon, S. Andermatt, N. Holmberg, G.K. Schenter, A. Hehn, A. Bussy, F. Belleflamme, G. Tabacchi, A. Glöß, M. Lass, I. Bethune, C.J. Mundy, C. Plessl, M. Watkins, J. VandeVondele, M. Krack, J. Hutter, CP2K: an electronic structure and molecular dynamics software package - Quickstep: efficient and accurate electronic structure calculations, J. Chem. Phys. 152 (2020), https://doi.org/10.1063/5.0007045.
[27] J. Vandevondele, M. Krack, F. Mohamed, M. Parrinello, T. Chassaing, J. Hutter, Quickstep: fast and accurate density functional calculations using a mixed Gaussian and plane waves approach, Comput. Phys. Commun. 167 (2) (2005) 103–128, https://doi.org/10.1016/j.cpc.2004.12.014.
[28] S. Goedecker, M. Teter, Separable dual-space Gaussian pseudopotentials, Phys. Rev. B, Condens. Matter Mater. Phys. 54 (3) (1996) 1703–1710, https://doi.org/10.1103/PhysRevB.54.1703.
[29] A. Druzhinin, D. Ariosa, S. Siol, N. Ott, B. Straumal, J. Janczak-Rusch, L. Jeurgens, C. Cancellieri, Effect of the individual layer thickness on the transformation of Cu/W nano-multilayers into nanocomposites, Materialia 7 (2019) 100400, https://doi.org/10.1016/j.mtla.2019.100400.
[30] P. Lazić, CellMatch: combining two unit cells into a common supercell with minimal strain, Comput. Phys. Commun. 197 (2015) 324–334, https://doi.org/10.1016/j.cpc.2015.08.038.
[31] F. Baras, O. Politano, Y. Li, V. Turlo, A molecular dynamics study of Ag-Ni nanometric multilayers: thermal behavior and stability, Nanomaterials 13 (14) (2023), https://doi.org/10.3390/nano13142134.