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Diffusion bonding of Cu atoms with molecular dynamics simulations

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ABSTRACT

Diffusion bonding of copper disks is an important step during the assembly of accelerating structures -the main components of power radio-frequency linear accelerators-. During the diffusion bonding copper disks are subjected to pressure at high temperatures. Finding the optimal combination of pressure and temperature will enable an accurate design of manufacturing workflow and machining tolerances. However, required optimization is not possible without good understanding of physical processes developed in copper under pressure and high temperature. In this work, the combined effect of temperature and pressure on closing time of intergranular voids is examined by means of molecular dynamics simulations. In particular, a nano-void of 3.5–5.5 nm in diameter representing a peak and a valley of surface roughness facing each other was inserted between identical copper grains. The simulations performed at T = 1250 K, the temperature used in experimental condition, and the 300–800 MPa pressure range indicated the dislocation-mediated enhancement of atomic diffusion leading to full void closure.

1. Introduction

The Compact LInear Collider (CLIC) [1] is a TeV-scale high luminosity linear electron-positron collider under development at CERN. CLIC uses a two-beam acceleration scheme in which normal conducting high gradient 12 GHz Accelerating Structures (AS) are powered via a high gradient Drive Beam. CLIC is foreseen to be built in stages [2] with a corresponding accelerator length from 11 to 50 km, for its last stage with a center of mass energy of 3 TeV, 20.760 two beam modules [3] are needed and in those 150.000 AS shall be assembled.

The present paper focuses on the needs of the radio-frequency (RF) copper disks [4] which are the main component of the AS (Fig. 1). Diffusion bonding method [5–7] has been identified as the most optimal way to join the copper disks interfaces without the need of filler metal and obtain clean and smooth surface, which is critical for the resistance at very high surface electric fields. The RF copper disks have micro-precision tolerances on one hand to guide high gradient (⩾100 MV/m) electromagnetic fields in ultra-high vacuum, while on the other hand to facilitate the joining process and result in a good bonded joint.

Machining tolerances [8] that are not critical for the RF performance (like the roughness in the interfaces) could be relaxed in order to bring the fabrication cost down. Even though there is already a development of AS, the diffusion bonding parameters currently in use (0.1 MPa applied pressure, temperature 1298 K −0.95 of the experimental melting point- during one and a half hours) have not been conclusively shown to be the optimal ones.

Several tests have been performed [9,10] with variable applied pressure and surface roughness aiming to find the best combination of the diffusion bonding parameters. The main aspects that were examined in former experiments is the preservation of the overall dimensions after the diffusion bonding and the quality of the final bonded joint in the interface of the RF disks with respect to the required micro-precision tolerances.

The atom-level simulations may elucidate the effect of diffusion bonding parameters on the quality of the bonded joint, i.e. the interface between two adjacent surfaces in order to redefine machining tolerance, i.e. surface roughness. Thus, molecular dynamics (MD) simulations could provide critical answers to something that remain inaccessible by experimental methods. Previously, by using MD simulations [11] the stability of voids in Cu with respect to the diffusion bonding procedure were examined. It was shown that the intergranular voids were thermally unstable and were filled up with atoms at the temperatures far below the melting point (T_m) due to enhanced diffusion in the grain boundaries (GB). On the other hand, the voids inside the grains (single crystals) were found to be thermally stable up to 0.94

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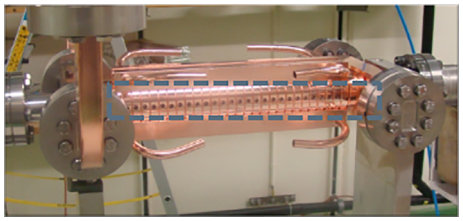


Fig. 1. Image of an Accelerating Structure (AS). The black dashed box highlights the pile of RF disks already bonded.

T_m.

This paper examines the combined effect of the applied pressure and temperature in the void's closing time like the diffusion bonding parameters. Provided the fact that the coexistence of GB and void create the aforementioned thermal instability and leads the voids to full closure with only the temperature application; in the current analysis voids are examined in the interface of identical grains.

2. Simulation procedure

Simulations were conducted using the LAMMPS software [12,13], while OVITO [14] was used for 3D-visualization. The embedded atomic method (EAM) [15] was used as the most suitable for the metallic bonds to calculate the interaction between the atoms. Considering the diffusion processes at high temperature, the Mishin potential [16] was chosen with a timestep of 1 fs. The predicted melting point of Cu according to this potential is 1327 K, which is very close to the experimentally determined value 1356.15 K.

The size of the simulation cells are presented in Table 1. Although we study the closing of the void placed in the grain boundary between the two grains, we chose to exclude additional degree of complexity related to the grain boundary diffusion, which depends on the misalignment of the adjacent grains. Both grains in the present simulations have identical orientation with the normal to the surface in the ⟨001⟩ crystallographic direction. Each simulation was divided in six subsequent steps. The targeted temperature was 1250 K and it was reached gradually in the three first steps. This temperature was targeted, since it had been found previously as the maximum temperature where a structure with identical orientation could remain stable.

A cylindrical void with a diameter of 3.5, 4, 4.5 and 5.5 nm was inserted during the forth step, and the periodic boundary along the z-axis was changed to non-periodic in order to apply the compressive pressure on the z-axis. Fig. 2 shows the configuration of the forth simulation step. Three atomic layers were fixed at the bottom and the top was left as an open surface. The system was then equilibrated again for 100 ps at the desired temperature using the Berendsen [17] thermostat with $\tau = 0.1$ ps, followed by the run in the micro-canonical ensemble.

The simulations were performed with the compressive uni-axial stress applied at the top (below the open surface) of the simulation cell. The tested stress range was 350–750, 300–800, 450–750 and 650–750 MPa for the 3.5, 4, 4.5 and 5.5 nm void sizes, respectively. These ranges had been selected based on the limitations of the central processing unit (CPU) time in a multicore machine. The pressure was

Table 1
Dimensions (nm) of the simulation box in the three directions for all the examined cases.

Directions	Void's diameter (nm)			
	3.5	4	4.5	5.5
x	11.3	13.0	14.3	17.3
y	1.8	1.8	1.8	1.8
z	16.5	13.0	17.5	18.5

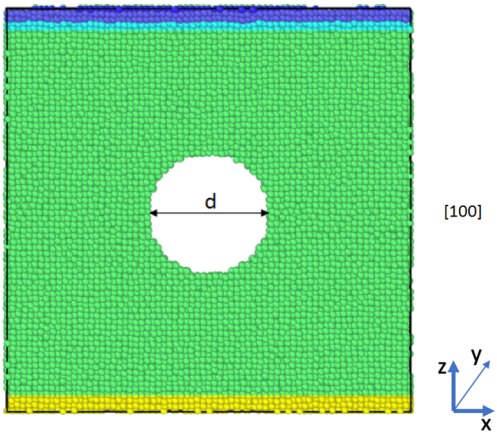


Fig. 2. Configuration of the 4th simulation step. Simulation box with Cu atoms in [100] orientation and a void in the middle with diameter 'd'. The yellow layer represents the fixed atoms, the light-black layer of atoms apply the compressive pressure and the black is the free surface.

applied in two steps on the layer below the free surface. During the fifth step the pressure was gradually increased from 0 up until the desired value was reached. The duration of this step at a constant rate of 10 MPa/ps depended on the pressure value that was examined. This rate had been determined after several trials as a compromise between the reasonably fast MD time-scales and any artificial rise of the pressure. In addition, the ramping rate had to be shorter than the total closing time. As a sixth step, the constant force was applied until the closure of the void.

In each case of applied pressure at least 100 runs were acquired. In the bigger void sizes like 4.5 and 5.5 nm only the higher pressure values were examined because of CPU processing limitations.

This paper examines the diffusion bonding parameters with molecular dynamics simulations. The interface of the two faces in contact and their roughness is represented with a circular nanovoid in different sizes.

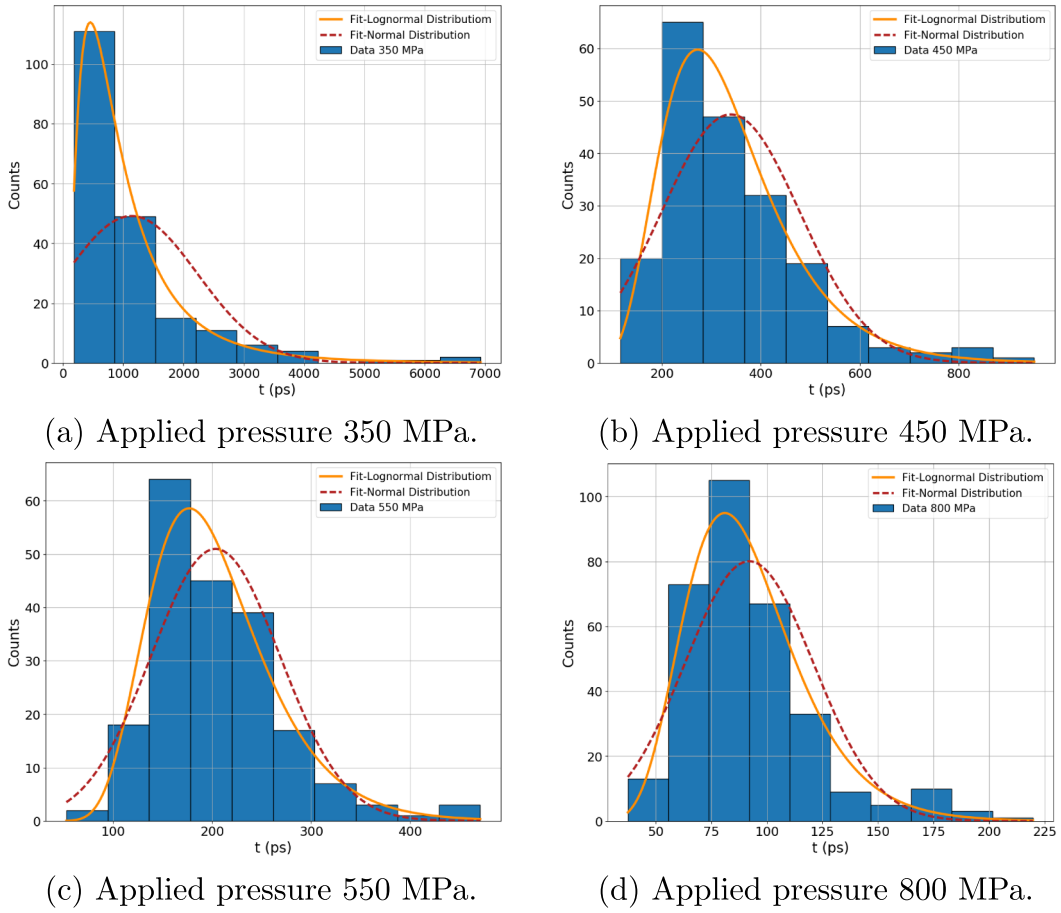
The applied temperature is the same as in the diffusion bonding conditions, while the impact of pressure is examined within a higher range than the real experiments – due to MD limitations -; aiming to extrapolate to a lower pressure regime.

3. Results

In the previous work [11], the voids within a single crystal have been found to be thermally stable up to the temperature of 1250 K, at least, within the MD time span. On the other hand, the voids placed between the grains with different orientation showed thermal instability, which was driving them to the full closure. The current paper aims to complete the picture of the most important parameters in the diffusion bonding process, by examining the impact of applied pressure along with high temperature in voids within a single crystal.

Fig. 3 presents the distributions of the closing time (ps) of 4 nm voids at applied pressures 350, 450, 550 and 800 MPa, respectively. The distributions were fitted with both, normal (dashed red curve in Fig. 3) and log-normal (solid orange line in Fig. 3) distributions. While both fits look similar, the log-normal distribution appears to capture the skewness of the distribution better. The fit results in Fig. 3 show that for high pressures, both distributions fit the data well, however, for the lowest pressure 350 MPa the log-normal distribution clearly fits the data better. This is also reflected in the mean values obtained with both distributions (Fig. 4a), for which the difference between the mean values obtained with the two different fits is clear at low pressures (Fig. 4b).

The voids of 3.5, 4.5 and 5.5 nm in diameter were examined for few pressure values. Fig. 5 presents the results of the closing time for voids



(a) Applied pressure 350 MPa. (b) Applied pressure 450 MPa.

(c) Applied pressure 550 MPa. (d) Applied pressure 800 MPa.

Fig. 3. Distributions of the 4 nm void's closing time (ps) at 1250 K and applied pressures 350, 450, 550 and 800 MPa respectively; fitted with log-normal and normal distributions. The solid orange lines represent the fitting with the log-normal while the dashed red lines the fitting with the normal distribution.

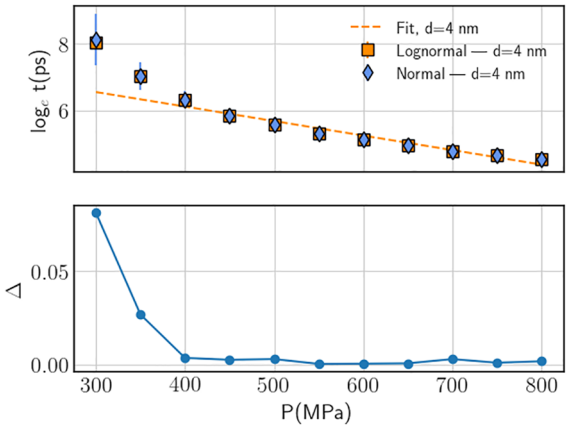


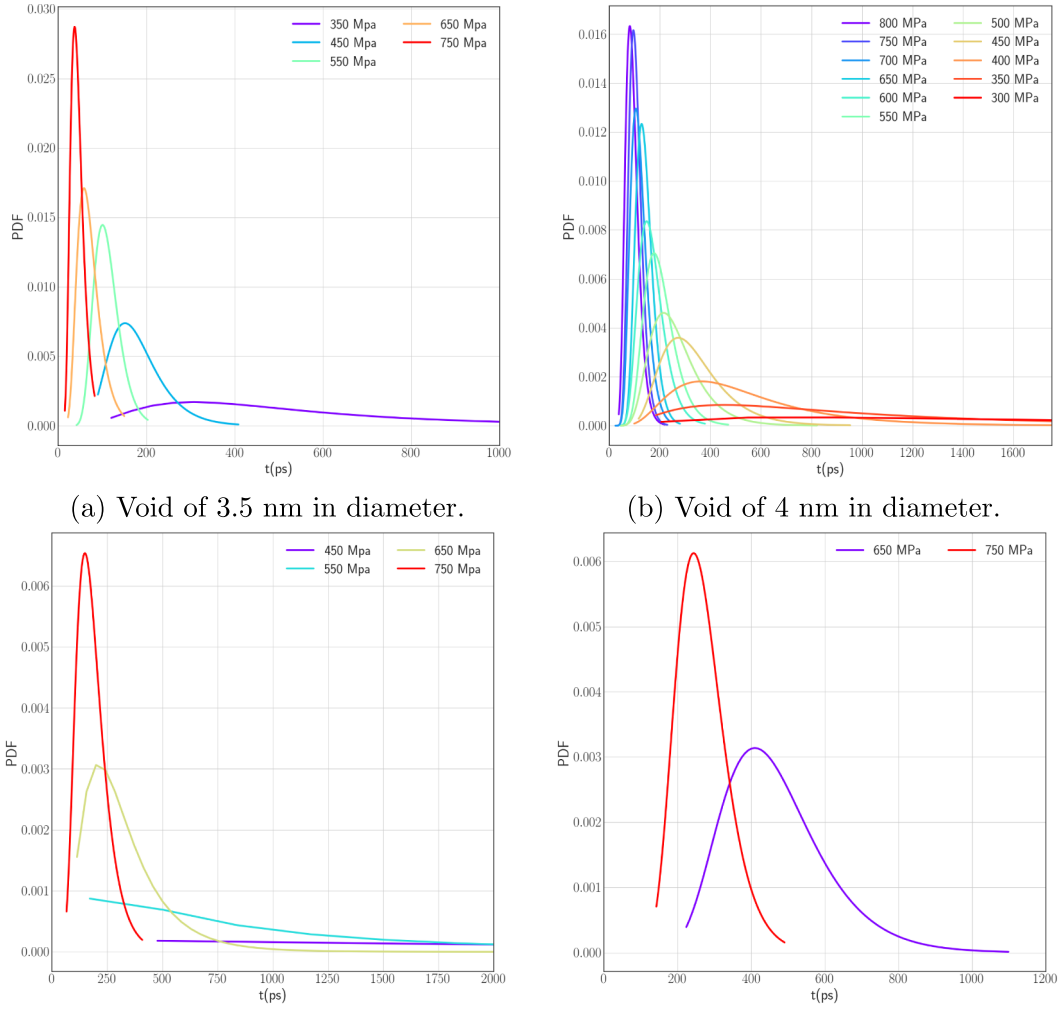
Fig. 4. Top: Mean values of the closing time versus the applied pressure for the 4 nm void at 1250 K. The squares represent the mean values which derive from a log-normal fitting of the raw data, while the diamonds from a fitting to a normal distribution. Bottom: Difference of the mean values between log-normal and normal distribution.

with diameter 3.5, 4, 4.5 and 5.5 nm fitted with log-normal distribution. The mean values of these distributions are plotted in Fig. 6 versus applied pressure in a semi-log plot similarly to Fig. 4.

4. Discussion

Based on Arrhenius equation as already suggested in [11] a linear fit is used to fit the mean values of closing times and is shown in Fig. 4 by the straight dashed line in the semi-log plot. The rationale behind this is that if the closing of the void proceeds via the diffusion jumps of atoms from the surface of the void. Linear fit of the logarithm of closing time versus applied pressure at a fixed temperature may confirm this assumption. The linear fit would imply that the applied uni-axial stress is translated into the hydrostatic pressure near the void surface, which is plausible to assume, since the surface of a nanometric void is molten at the studied high temperature of 1250 K. Although the fitting follows closely the logarithms of the mean values of $t_{closing}$ at high pressures, a clear deviation from the straight line in this graph appears when the external pressure is reduced. More precisely, the deviation takes place at the pressures around 450 MPa. The same fit was attempted for all examined void sizes and the results are shown in Fig. 6. In this plot, the deviation from linear behavior for a smaller void begins at approximately the same pressure of 4 nm void (450 MPa), while for larger voids, the results are less conclusive because of smaller statistics, which was obtained for these cases due to CPU time limitations. However, it is consistently seen that the increase of skewness of distributions at a given pressure in Fig. 5c and d coincide with deviation from the linear behavior of $log(t_{closing})(p)$ in Fig. 6.

To understand the nature of this deviation, it is necessary to analyse the mechanisms of the processes leading to filling of the void. The diffusion processes are well-described by a 'random walk' model, where every atom that ended up inside of the void can be considered as an independent random walker. Hence, the total time needed for the void to be filled in, can be found as an arithmetic sum of all the random walkers that jumped independently into the void, $t_{closing} = N \cdot t$. Here t is the mean waiting time for an atom to jump into the void and N is the number of atoms (random walkers) needed to fill the void. The sum of



(a) Void of 3.5 nm in diameter. (b) Void of 4 nm in diameter.

(c) Void of 4.5 nm in diameter. (d) Void of 5.5 nm in diameter.

Fig. 5. Probability density function of the log-normal distributions of the voids closing time versus applied pressures; for the voids with diameter 3.5, 4, 4.5 and 5.5 nm respectively.

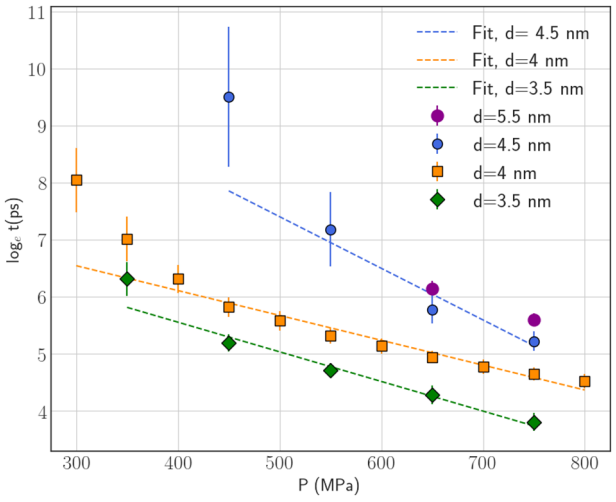


Fig. 6. Mean values of the voids closing time (ps) versus the applied pressure for all void sizes at 1250 K.

all t results in a normally distributed value of the total time needed to close the void, $t_{closing}$. Therefore, the Arrhenius plot for $t_{closing}$ as a function of $(1/T)$ is linear, as was shown in [11]. Under an external pressure as in the current simulations, if the atoms fill the gap in a random walk as well, and the difference in $t_{closing}$ is expected only due to the effect of applied external pressure on the activation barrier, linear behavior would sufficiently well describe the dependence of $t_{closing}(p)$. In this case, the deviation from the line in Fig. 4 would not be observed. The appearance of the puzzling deviation at lower pressure motivates obtaining a deeper understanding of the filling process.

It is natural to assume that deviation in the behavior of any process may be caused by changing of the mechanism governing this process. Under significant pressure and high temperature, the formation of more complex structural defects [18] (dislocations and stacking faults) is expected. In the face-centered cubic lattice (FCC) lattice, such defects can be identified as Hexagonal Closest Packed (HCP) atoms, which form stacking faults and coherent twin boundaries and are therefore important for the identification of partial dislocations. Thus, Dislocation Extraction Algorithm (DXA) is performed with OVITO [19]. The number of HCP atoms were analyzed for the 4 nm void case at the last step of the simulation until the void's full closure (Fig. 7). The error bars shown in Fig. 7 derived after analyzing twenty cases of each examined pressure, except the 450 MPa case where hundred cases were considered. Fig. 7 shows a linear relation between the number of HCP atoms versus the applied pressure and hence a gradual increase of average atoms involved in formation of stacking faults.

Atoms in the stacking faults [20] migrate rapidly towards the surface of the void due to the image force supplying more than one atom at a time to fill in the void. The higher the pressure, the larger the stacking

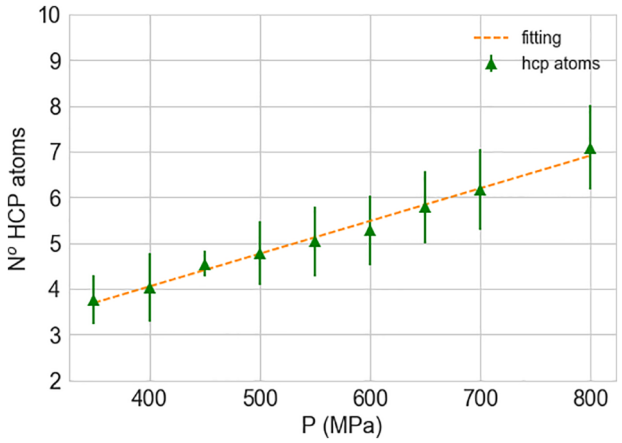


Fig. 7. HCP atoms of the 4 nm void case plotted versus the applied pressure. The dashed line is a linear fit to the data.

faults, and the more atoms are brought in, to fill the void. Since the formation of the stacking faults is a probabilistic event with the probability increased with the applied pressure, the size of the stacking faults will be normally distributed. On the contrary, for low pressures (below the pressure 450–500 MPa), the stacking faults form less prominently, increasing the uncertainty of how many atoms jumped into the void and the dislocation nucleation becomes a stochastic phenomenon which is described better by a log-normal distribution.

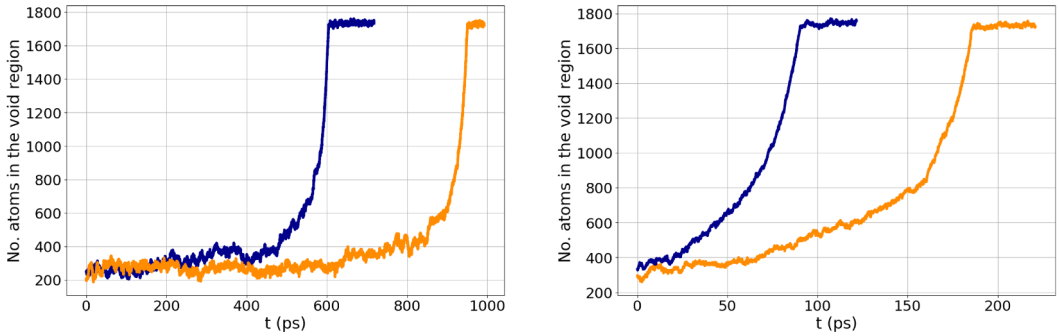
It is worth analysing now the stresses in the void region. The critical resolved stress which is actually the minimum stress required to initiate a slip [21] is estimated between the theoretical ideal value of 1/6G (where G is the shear modulus of copper equal to 50 GPa [22]) and the more accurate based on physical considerations of 1/30G, which results in the range of 1.7–8 GPa. Decreasing this value further due to by the high ambient temperature used in the simulations by 75% as it was shown in [22], and the critical resolved shear stress drops to the value of 425 MPa. Finite element analysis had been conducted using ANSYS Workbench as shown in Appendix to analyse the stress concentration around a void under uni-axial compressing pressure. The maximum normal stress appears always [23] at the surface of the void at the vertical midpoints, and is three times higher than the applied stress (Fig. 11). The shear stress found to be about 85% (Fig. 13) of the pressure applied at the surface. Considering the pressure region where the deviation from linearity (450–500 MPa) takes place, the maximum shear stress for those would be very close to the theoretical estimated value (425 MPa). This value is surprisingly close to the estimated value of the critical resolved shear stress, which confirms the switch of the mechanisms from the driven by direct formation of dislocations under very high pressures and probabilistic formation of dislocations under the shear stress below the critical value. In both cases the $t_{closing}$ is described by the log-normal distribution, however, above the critical resolved shear stress ($>$ 425–450 MPa), it is closer to normal, since the size and the frequency of the formed dislocations are much closer to one another.

Fig. 8 examines two extreme cases of the same distribution for the 4 nm void, when pressure of 350 MPa (on the left) and 700 MPa (on the right) is applied. Fig. 8 shows the atoms filling up the void until the full closure. The *y*-axis is identical for both pressure cases, since the void size is the same. In the *x*-axis there is a difference in scale, due to faster closing of the void for the higher pressure. Qualitatively, the two examined cases at each pressure show the same exponentially accelerated closing behavior only with different proportionality factors. This suggests that there is only one diffusion mechanism driving the two voids between the two extreme cases and the observed discrepancy is due to random motion, however, this random motion is not driven by a single atom, but by clusters of atoms whose size is also random.

For reasons of comparison, the distribution of the closing time is examined in a 3.5 nm void placed in a grain boundary (GB) (Fig. 9a). The effect of the GB was investigated by setting up the simulation cell to mimic separate grains of poly-crystalline Cu, which face the GB with crystallographic orientations [1 0 0] at the bottom and [1 1 0] at the top with the mis-orientation angle $\theta = 45°$ along the z direction. The details of the cell construction and its equilibration at the desired temperature can be found elsewhere [11]. The examined temperature equals 1250 K, as in aforementioned simulations, however no pressure is applied. In this case, the GB was used to enable the closing of the void within the MD time span. The resulted distribution after 100 runs is shown in Fig. 9b where both log-normal (continuous line) and normal (dashed line) distributions are fitted. This comparison implies that the distribution of the atoms filling up the void at 1250 K is described better by a log-normal distribution independent from the crystallographic structure (existence or not of a GB). A quantitative comparison between the distributions of the 3.5 nm void case without applied pressure and the case of the lowest applied pressure is not relevant. In the first case, the presence of the grain boundary enhances the diffusion, compared to the case where the single crystal is subjected to volume diffusion with the presence of applied pressure at the same temperature. However, the result shows that log-normal distribution of closing times is also observed without pressure, but at very high temperatures when the spontaneous formation of stacking faults in FCC structure is possible. Hence, this result confirms the importance of the present study indicating that to understand the mechanisms leading to the closure of the internal voids during the diffusion bonding at high temperatures, the dislocation-mediated mechanism must not be overlooked.

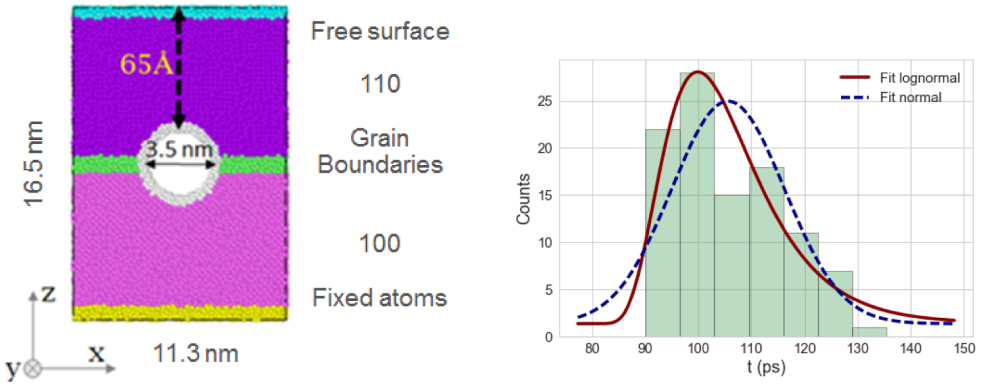
5. Conclusions

The paper examines the effect of applied pressure and temperature in the void's closing time, as the diffusion bonding parameters. The examined voids of diameter 3.5, 4, 4.5 and 5.5 nm are positioned in the



(a) Applied pressure: 350 MPa. (b) Applied pressure: 700 MPa.

Fig. 8. Atoms filling up the empty space of the void with diameter of 4 nm at 1250 K when pressure of 350 MPa (on the left) and 700 MPa (on the right) is applied, for two different runs that differ only in the random atom fluctuations.



(a) Simulation's Setup. (b) Fitting on the distribution.

Fig. 9. On the left: Image of the simulation setup conducted for a 3.5 nm void in the interface of two crystals, with zero pressure at 1250 K. On the right: Distribution of the closing time fitted with log-normal distribution (continuous line) and normal distribution (dashed line).

interface of identical grains. The simulation temperature at the last step reaches 1250 K and the examined pressure range is 300–800 MPa.

The distributions of the closing times for different pressure values could be fitted both with normal and log-normal fitting. Nevertheless, the log-normal captures the skewness and fits the data better, especially at the lower examined pressure values. The linear fitting suggested earlier [11] fails to fit perfectly the logarithms of the mean values of the closing time, since at the examined pressure range additional phenomena than pure diffusion process appear and thus the Arrhenius plot of $t_{closing}$ is not sufficient to describe the process.

HCP atoms and stacking faults are present in the examined conditions and become more uniform in size with increase of the pressure resulting in a normal distribution and in a better linear fit at higher pressures. Lowering of the pressure leads to a reduction of the shear stress, which results in a more stochastic behavior of dislocation nucleation at the places where the highest shear stress appears (Fig. 13) and hence more random distribution in the number of atoms which jump into the void. Although the $t_{closing}$ is log-normally distributed, the difference between the number of atoms brought in the void at a time by the dislocation is so small above the resolved shear stress that the lognormal distribution of $t_{closing}$ for the external pressures above 450 MPa appears in shape much closer to the normal distribution.

A detailed study in the lower regime of pressure values is highly encouraged for future studies.

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.

Acknowledgements

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Appendix A

FEA calculations were conducted in order to demonstrate the stress concentration around the void.

A plate of copper is used with a void in its center as shown in Fig. 10. The dimensions of the plate were defined by translating the nano-meter scale of the smallest simulation box (Table 1) to millimeter scale. The boundary conditions are as in the MD simulations, fixed bottom face and applied compressing pressure (for example 100 MPa) on the top face. Linear periodic boundary (like periodic boundaries in MD) is applied through

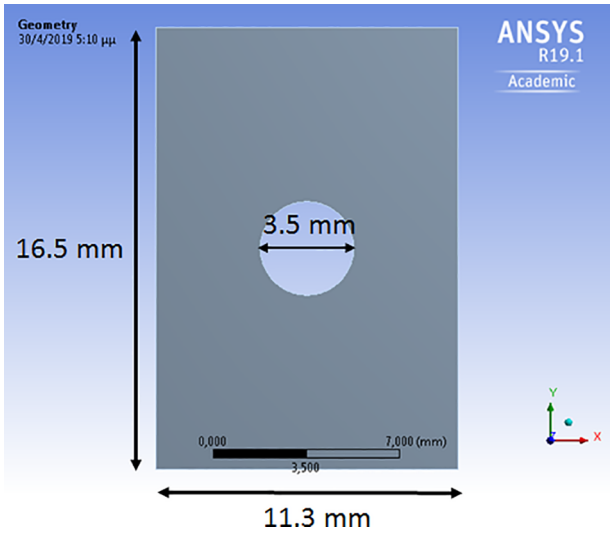

Fig. 10. Geometry used for the FEA simulations.

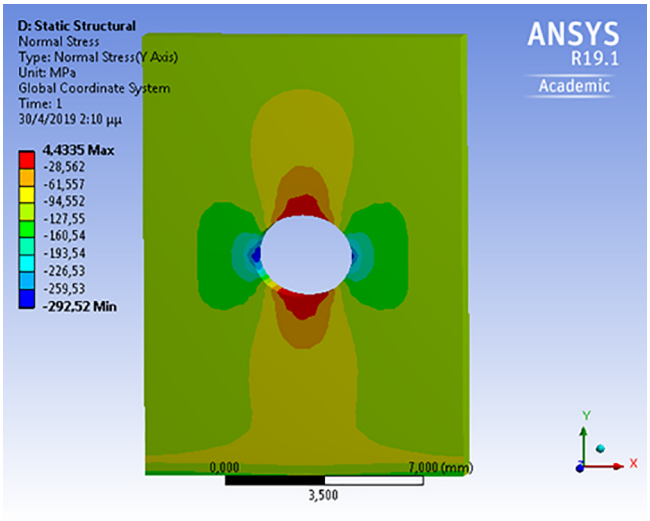

Fig. 11. Normal stress on the y-axis.

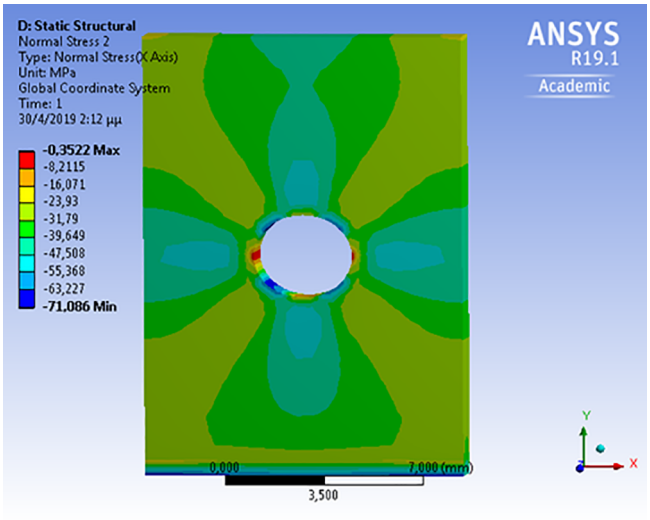

Fig. 12. Normal stress on the x-axis.

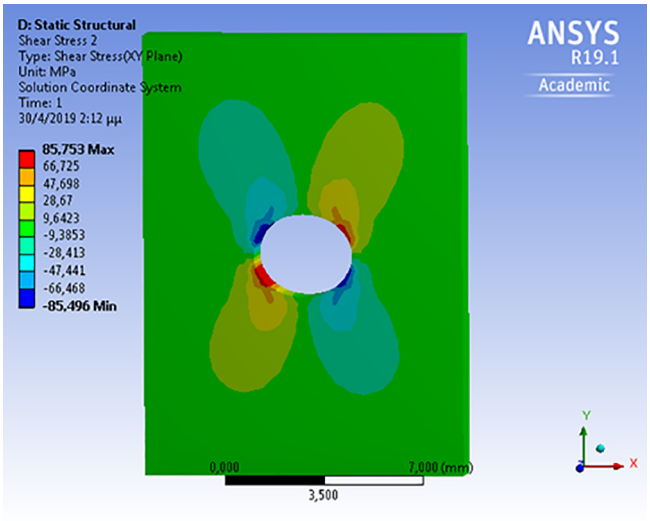

Fig. 13. Shear stress on the xy-plane.

symmetry, along the x-axis of the copper plate. In z-axis we didn't apply linear periodic since this feature supports only a single direction for the entire model (more than one direction is not supported). Through this calculation the normal and shear stresses are extracted and are shown in Fig. 12, 11, 13.

From Fig. 11 we validate that the $\sigma_{max} = -292$ MPa (due to compression) appears in the sides of the void and is three times higher than the applied pressure (100 MPa). Also it is shown that there is a normal stress of -70 MPa in the direction vertical to the applied pressure due to Poisson ratio (periodic boundary condition in lateral directions) and a shear stress of -85 MPa on the XY plane. Both σ_x and τ_{xy} components are lower than 1/3 of the applied pressure, therefore their effect on the void's closing time would be less significant.

Appendix B. Supplementary data

Supplementary data associated with this article can be found, in the online version, at https://doi.org/10.1016/j.rinp.2019.102890.

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