

1 **Origins of ductile plasticity in a polycrystalline**  
2 **gallium arsenide during scratching: MD**  
3 **simulation study**

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16  
17 **Abstract**

18 This paper used molecular dynamics simulation to obtain an improved understanding  
19 of the ductile plasticity in polycrystalline gallium arsenide (GaAs) during its  
20 nanoscratching. Velocity-controlled nanoscratching tests were performed with a  
21 diamond tool to study the friction-induced deformation behaviour of polycrystalline  
22 GaAs. Cutting temperature, sub-surface damage depth, cutting stresses, the evolution

23 of dislocations and the subsequent microstructural changes were extracted from the  
24 simulation. The simulated MD data indicated that the deformation of polycrystalline  
25 GaAs is accompanied by dislocation nucleation in the grain boundary leading to the  
26 initiation of plastic deformation. Furthermore, a dual slip mechanism was observed as  
27 an important factor driving plasticity in poly GaAs in sharp contrast to a single GaAs.  
28 The magnitude of cutting forces and the extent of sub-surface damage were both  
29 observed to reduce with an increase in the scratch velocity whereas the cutting  
30 temperature scaled with the cutting velocity. As for the depth of the scratch, an increase  
31 in its magnitude increased the cutting forces, temperature and damage-depth. A  
32 phenomenon of fluctuation from wave crests to wave troughs in the cutting forces was  
33 observed only during the cutting of polycrystalline GaAs and not during the cutting of  
34 single-crystal GaAs.

35

36 **Keywords:** Polycrystalline gallium arsenide; MD simulation; Grain boundary;  
37 Dislocation nucleation

38

## 39 **1 Introduction**

40 Gallium arsenide (GaAs) has emerged as a favourable choice as a III-V direct bandgap  
41 semiconductor due to its applications in 5G communication devices [1]. GaAs (which  
42 resides in a Zinc-blende structure) possesses superior properties to silicon, for instance,  
43 GaAs has a higher saturated electron velocity and higher electron mobility, allowing  
44 GaAs transistors to function swiftly at frequencies over 250 GHz. Owing to their wider  
45 energy bandgap, GaAs devices are relatively insensitive to overheating which makes

46 them less noisy while operating at higher frequencies in electronic circuits and that is  
47 where they outbid silicon devices. GaAs can be grown as a single crystal using methods  
48 such as the vertical gradient freeze method, the Bridgman-Stockbarger technique, or  
49 the Liquid encapsulated Czochralski growth process. Parallel to this, the use of  
50 polycrystalline GaAs as thin films is quite popular. Films of GaAs can be grown by  
51 chemical vapour deposition (by annealing an amorphously grown film), or by using  
52 molecular beam epitaxy (MBE). The processing cost of polycrystalline GaAs is lower  
53 than the processing cost of single crystal GaAs [2] and this allows polycrystalline GaAs  
54 to find wider applications in the field of solar cells [3][4], imaging detectors [5],  
55 microwave and optoelectronic devices [6].

56 Prior work suggests that poly and single crystals of silicon [7][8] and silicon carbide  
57 [9] showed differences in the incipient plasticity and material removal mechanism,  
58 although the fundamental reasons behind these differences were not immediately clear.  
59 The microstructure of material (such as grain boundaries and defects) also influences  
60 the Schottky barrier height. There are knowledge gaps like these that prompted the  
61 authors to investigate the mechanical deformation of polycrystalline GaAs using  
62 molecular dynamics (MD) simulation. As such, recent advances made in the  
63 computation hardware now offer the possibility [10] to use MD simulations as an  
64 advanced digital nano manufacturing tool. The remaining sections of the paper discuss  
65 the scratch forces, sub-surface damage, peak cutting temperature, cutting stresses in a  
66 polycrystalline substrate benchmarked against a single crystal GaAs substrate.

67

## 68 **2 MD simulation methodology**

### 69 *2.1 MD simulation model*

70 An orthogonal MD simulation nanoscratching model for cutting a polycrystalline GaAs  
71 was developed using the Voronoi site-rotation algorithm (see figure 1 and figure 2(a)).  
72 The diamond scratching tool was modelled with a negative rake angle of  $-25^\circ$  and a  
73 clearance angle of  $10^\circ$ . The polycrystalline GaAs workpiece was built by employing  
74 the AtomsK software [11] using the Voronoi algorithm [12][13]. The Voronoi site-  
75 rotation method generates a polycrystalline structure by joining the normals of the line  
76 of random discrete points at the crystal boundary and containing the growing random  
77 oriented crystal seeds. As shown in Fig. 2(b), the polycrystalline GaAs workpiece was  
78 divided into three regions of atoms i.e. Newtonian atoms (yellow and red color atoms),  
79 thermostat atoms (blue color atoms) and boundary atoms (green color atoms). Prior to  
80 cutting, the GaAs workpiece (containing 14 grains) was equilibrated for about 100 ps  
81 using the Nose-Hoover method [14] in LAMMPS (Large-scale atomic/molecular  
82 massively parallel simulator) [15]. Visualization and analysis were performed using  
83 Visual molecular dynamics (VMD) [16] and Open Visualization Tool (OVITO)  
84 softwares [17]. The detailed parameters used for the model development are shown in  
85 Table 1.

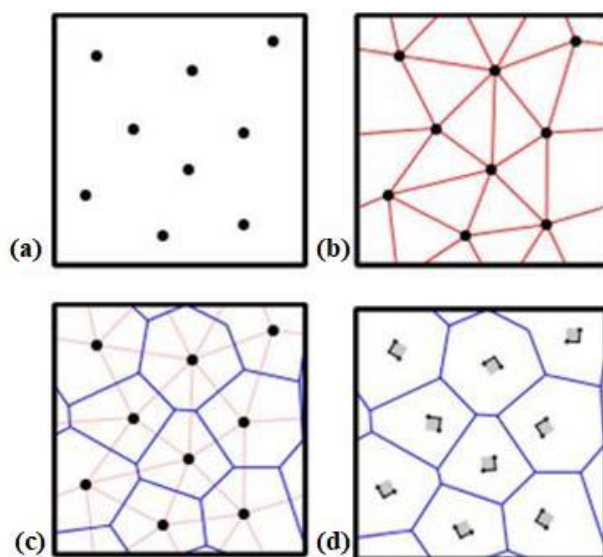
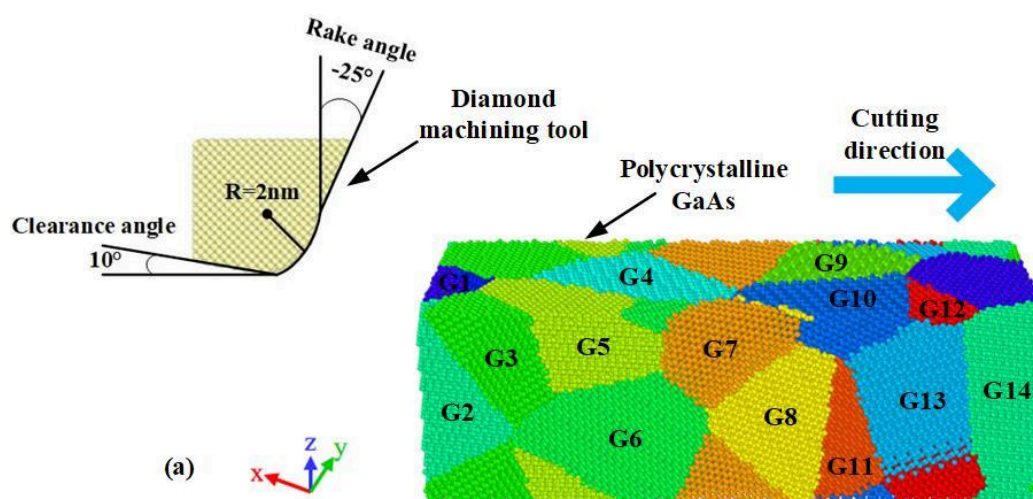


Fig. 1. Voronoi site-rotation illustration showing random points.

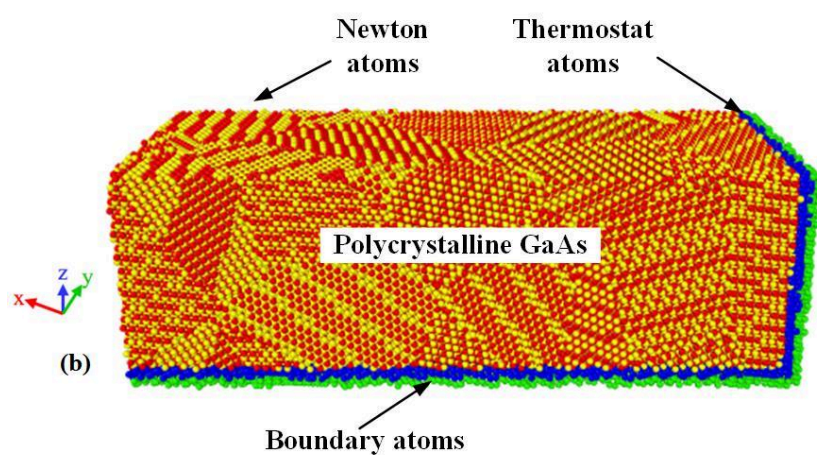
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Fig. 2. Nanoscratching model of polycrystalline GaAs showing different grains and tool description.

92

**Table 1:** Simulation parameters used to develop the MD simulation model

GaAs substrate dimensions	30.8 nm × 10.0 nm × 13.4 nm (X, Y and Z direction)
Number of atoms in the polycrystalline GaAs	184285 (total 14 grains)
Scratching tool	Diamond cutting tool (rigid)
Number of atoms in the tool	12085
Tool rake angle	-25°
Tool clearance angle	10°
Tool edge radius	2 nm
Equilibrium lattice constant of GaAs	5.78 Å (Zinc blende lattice structure)
Diamond lattice constant	3.57 Å (Diamond cubic lattice structure)
Width of cut	2.86 nm
Depth of cut	Was varied (0.5 nm, 1 nm and 2 nm)
Scratch velocity	Was varied (100 m/s, 200 m/s and 400 m/s)
Scratching distance	12 nm
Equilibration temperature	300 K
Timestep used for MD calculation	1 fs

93

## 94 *2.2 Selection of potential energy function*

95 The choice of potential function can make a significant difference on the accuracy of  
96 MD results. It is important to choose a robust potential especially when it concerns  
97 studying aspects of fracture, wear and plasticity of a material. In this investigation, the  
98 cutting of GaAs with a diamond tool required describing the interactions between and  
99 among three types of atoms namely, Ga, As and C atoms. Due to the unavailability of a  
100 single many-body potential parameterized to describe all these atoms, a hybrid scheme  
101 was employed here in a hybrid/overlay scheme offered by LAMMPS. For the sake of  
102 brevity and avoiding repeated information, the details of the potential function (which  
103 is readily available from the respective papers) are not repeated here, but generally

104 speaking, the covalently bonded interactions of C-C and the Ga-Ga, As-As and Ga-As  
105 interactions were all described by the analytical bond order potential developed by the  
106 research group of Albe et al. [18][19]. As for the cross interactions between the atoms  
107 of the diamond tool and the Gallium Arsenide workpiece (Ga-C and As-C), a Ziegler-  
108 Biersack-Littmark (ZBL) potential function [20] (pair\_style zbl in LAMMPS) was used  
109 which simply requires the atomic number and cut off parameters as an input.

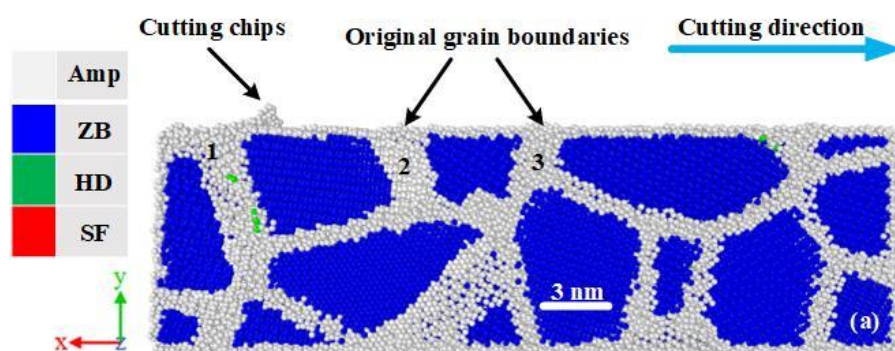
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### 111 **3 Results and discussions**

#### 112 *3.1 Microstructural changes*

113 Taking a test case of cutting depth of 2 nm and scratch velocity of 200 m/s, figure 3  
114 shows a simulation output wherein blue color atoms, white color atoms, green color  
115 atoms and red color atoms represent the perfect zinc blende (ZB) structure, amorphous  
116 (Amp) structure, hexagonal diamond (HD) structure and stacking faults (SF)  
117 respectively. The grain boundaries that were analyzed are marked by number 1, 2, and  
118 3, respectively.

119





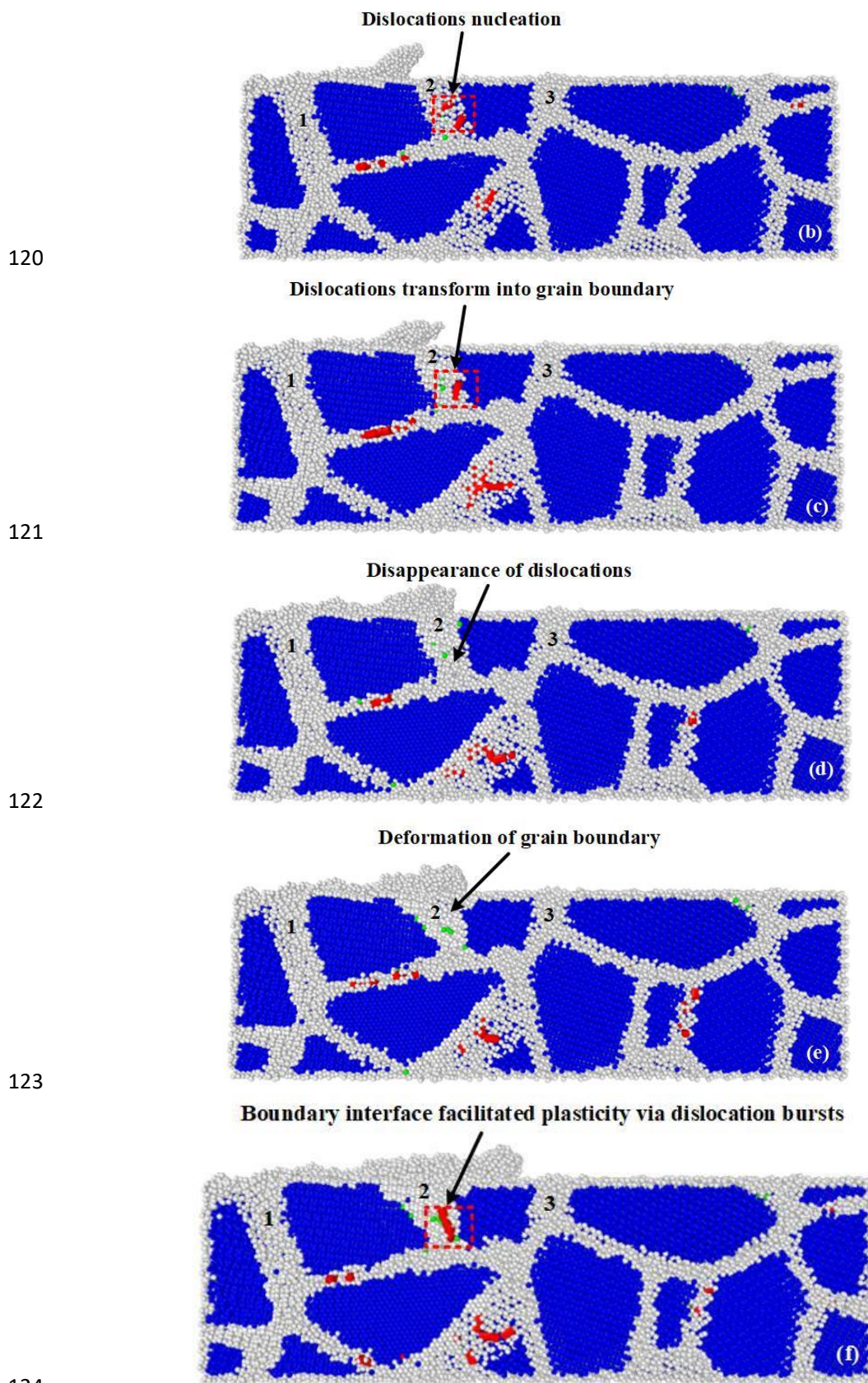


Fig. 3. Cross-sectional image of the polycrystalline GaAs (tool is kept hidden for visualization and cutting is performed at a depth of 2 nm and scratch velocity of 200 m/s). The snapshots are taken at cutting



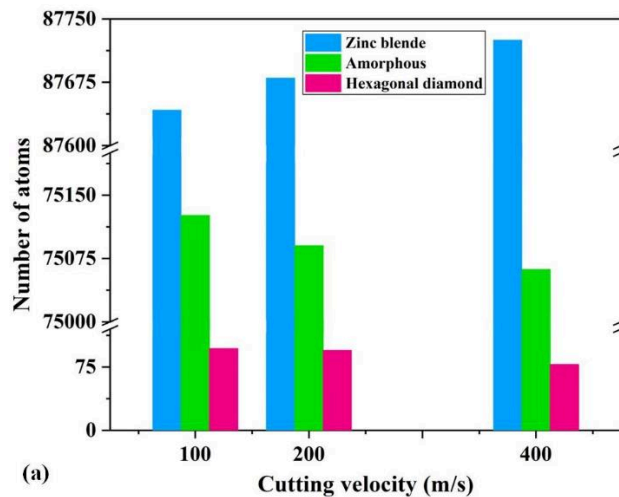
127 distances (a) 3 nm, (b) 6 nm, (c) 7 nm, (d) 8 nm, (e) 9 nm and (f) 12 nm. Pictures were processed using  
128 OVITO.

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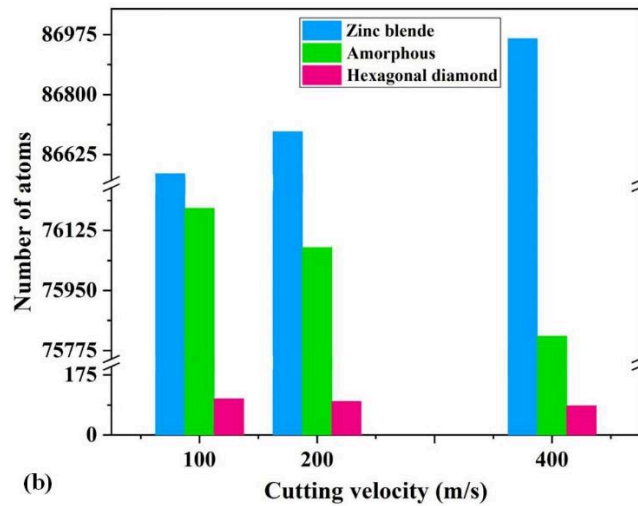
130 As shown in Fig. 3(a), the grain boundaries marked by 1, 2 and 3 were chosen as the  
131 sites of analysis for post-processing visualization of the dislocation and stacking fault  
132 structures using the second nearest neighbor scheme relying on an extended common  
133 neighbor analysis implemented in OVITO [21]. Fig. 3(b) highlights the initiation of the  
134 nucleation of dislocations at several places in the grain boundary 2 (GB 2). With  
135 subsequent tool travel, i.e. at the cutting distance of 7 nm, a part of the dislocations  
136 created at a cutting distance of 6 nm started to transform to grey color atoms and became  
137 a part of GB 2. Subsequently, the dislocations within GB 2 disappeared and transformed  
138 into a grain boundary marked by grey color atoms at the cutting distance of 8 nm shown  
139 in Fig. 3(d). Meanwhile, a small number of green atoms were found present in the grain  
140 boundaries. At the cutting distance of 8 nm, the GB 2 widens and became thicker as  
141 may be seen in Fig. 3(e). Finally, as shown in Fig. 3(f), a large dislocation burst  
142 appeared in the GB 2 at the cutting distance of 12 nm, and a few grey color atoms  
143 transformed into red color atoms. The observation reported here remains consistent in  
144 all the simulation test cases.

145 Meanwhile, the evolution of structural changes in polycrystalline GaAs was quantified  
146 as a function of cutting velocity at various depths of scratch (see Fig. 4). It must be  
147 noted here that the ABOP potential function used in this study does not predict the  
148 energy differences between the cubic diamond and hexagonal closed packed diamond  
149 and hence the observation of hexagonal diamond in this study is a mere reflection on

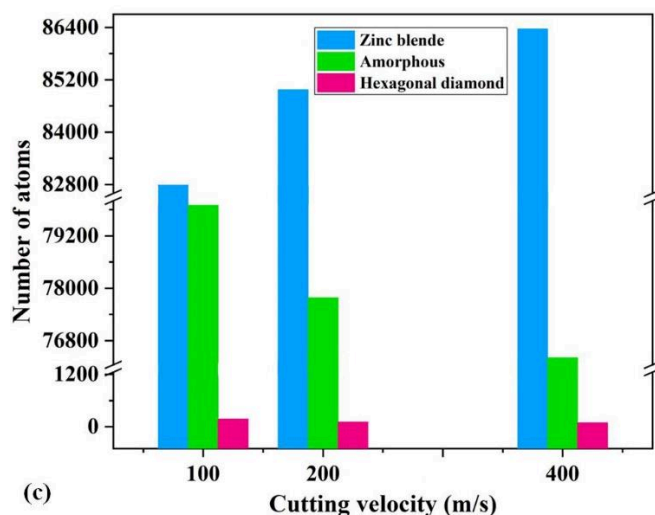
150 the faulted diamond cubic structure [22]. Overall, results in figure 4 show that a higher  
151 cutting velocity leads to a reduced degree of structural transformation in the material.  
152 Additionally, it was observed that all such microstructural transformations initiate  
153 preferentially in the grain boundaries. It implies that grain boundaries are preferred sites  
154 of nucleation of dislocations during the scratching of a polycrystalline substrate.



155



156



157

158 **Fig. 4.** The evolution of microstructure changes in polycrystalline GaAs during nanoscratching process

159 with various cutting velocities under cutting depth of 0.5 nm (a), 1 nm (b) and 2 nm (c). Note here that

160 the occurrence of the formation of hexagonal diamond is a mere artefact since the potential function used

161 in this study does not distinguish energy differences between cubic and hexagonal phases.

162

163 *3.2 Analysis of dislocation nucleation*

164 Fig. 5 shows the details of dislocation nucleation. According to the three-dimensional

165 (3D) images, the nucleation of dislocations (marked by red color atoms) occurred in the

166 grain boundaries, which is consistent with the two-dimensional (2D) images shown

167 earlier in Fig. 3. As no dislocations were found inside of the individual grains of

168 polycrystalline GaAs, it indicated that the grain boundaries are softer than the grains

169 and deform swiftly. This phenomenon is in accordance with the recently reported work

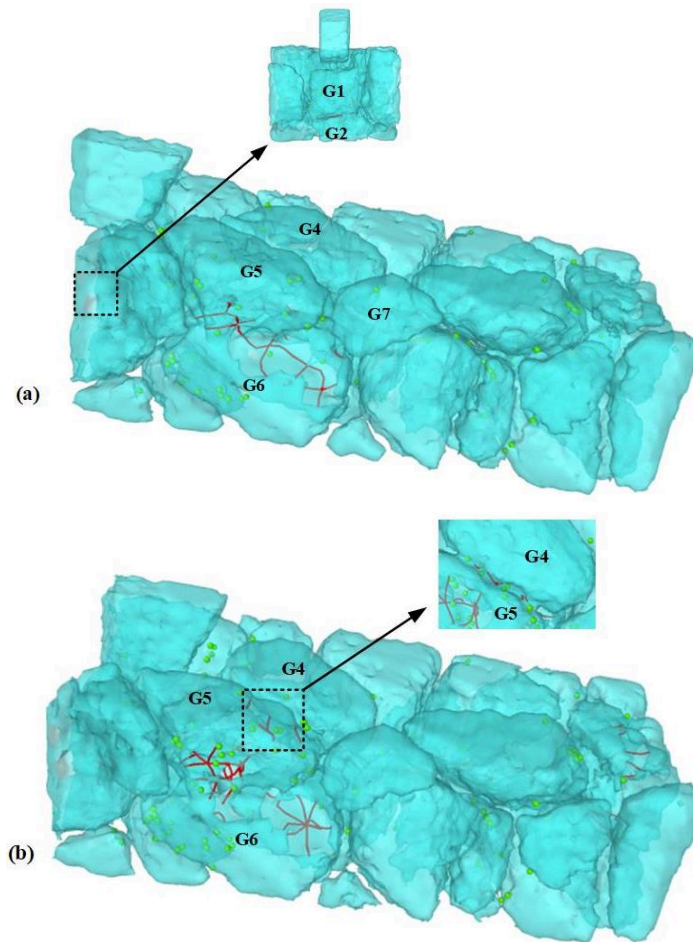
170 on polycrystalline silicon carbide material [23]. Additionally, when the diamond tool

171 penetrated the polycrystalline GaAs at 3 nm (see Fig. 5(a)), the two clusters of the

172 dislocations were found in G1-G2 and G5-G6, respectively. Subsequently, the

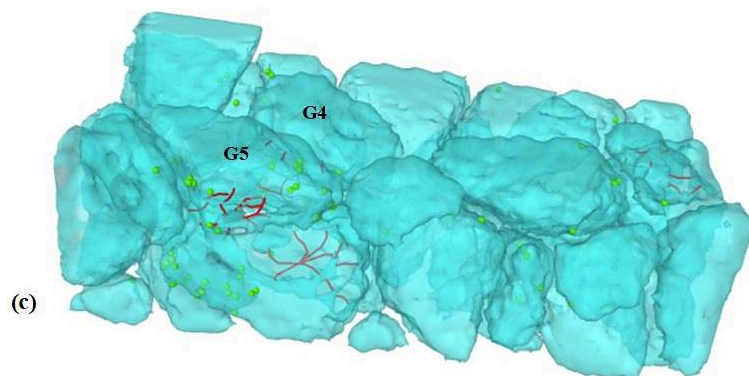
173 dislocation nucleation diffused through G4-G5 and the right corner of the

174 polycrystalline GaAs workpiece, as illustrated in Fig. 5(b). In accordance with Fig. 5(c)  
175 and Fig. 5(d), the dislocation nucleation kept reappearing when the diamond tool passed  
176 through the edge of the grain boundary between G4 and G5. When the diamond tool  
177 started to penetrate the grain boundary between G4 and G5, there was no dislocation  
178 nucleation in G4-G5 (see figure 5(e)). The dislocation nucleation was distributed across  
179 the G5-G6 and G7-G8-G9-G10-G11-G13. Finally, the dislocation nucleation  
180 reoccurred in the G4-G5, as showed in Fig. 5(f), while the diamond tool cuts the grain  
181 boundary between G4 and G5.

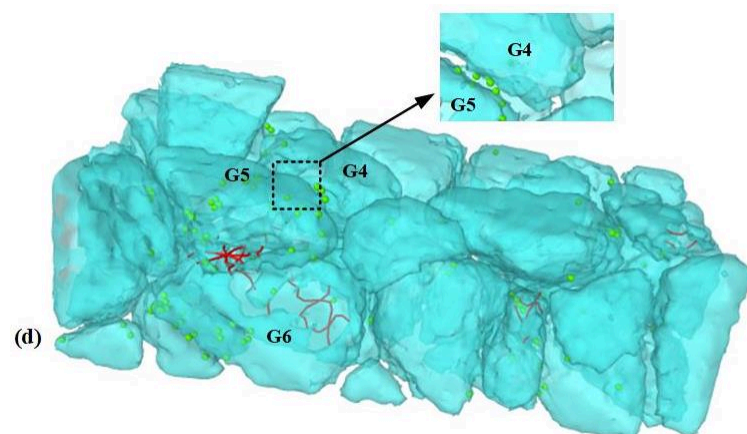


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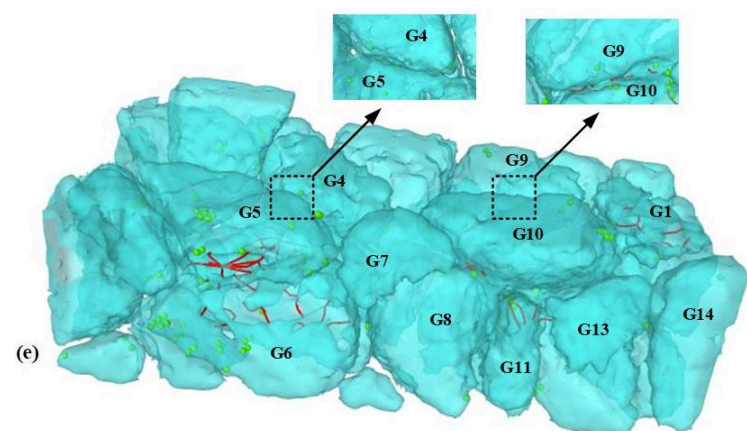
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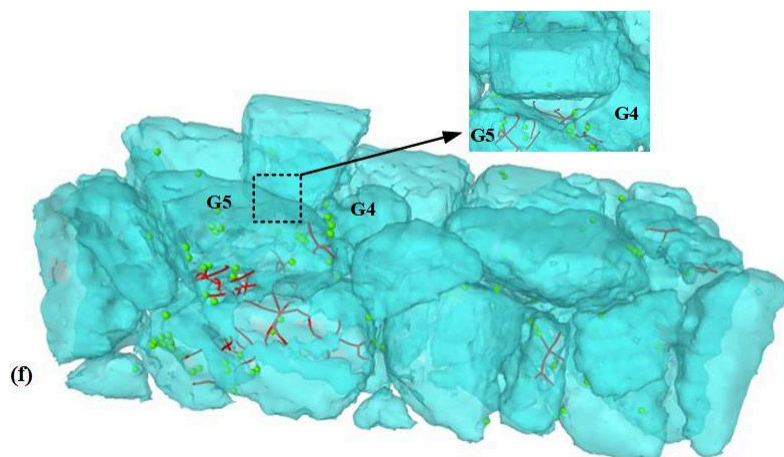
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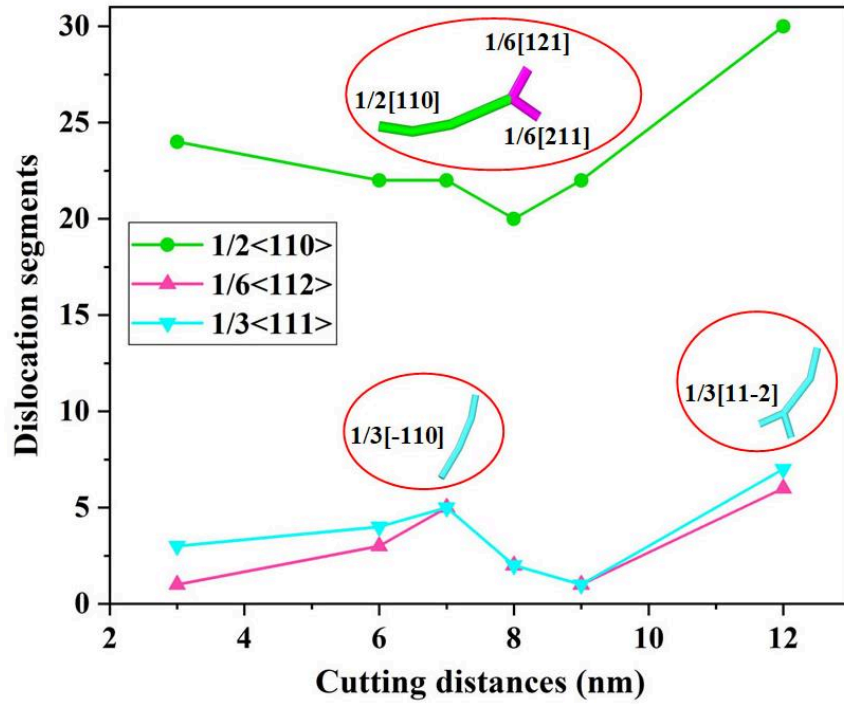
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188 **Fig. 5.** The movement of dislocations in the polycrystalline GaAs at (a) 3 nm (b), 6 nm (c), 7 nm (d), 8  
189 nm (e), 9 nm and (f) 12 nm.

190 In terms of the quantitative analysis, the number of dislocation segments extracted from  
191 the MD data is shown in Fig. 6. It can be seen that the presence of  $1/2\langle 110 \rangle$  type  
192 dislocations dominated others which was responsible for the incipient plasticity  
193 observed in the polycrystalline GaAs. The two other dislocations of type  $\frac{1}{6}\langle 112 \rangle$  and  
194  $\frac{1}{3}\langle 111 \rangle$  were also present and were of the same length for the duration of cutting studied  
195 here. During the simulation, the dislocation with  $1/2[110]$  Burgers vector was observed  
196 to split into two Shockley partials with one having  $1/6 [121]$  Burgers vector and the  
197 other having  $1/6 [211]$  Burgers vector. The dissociation reaction can be represented as  
198  $1/2 [110] = 1/6 [121] + 1/6 [211]$ .

199 Also, the  $1/3\langle 111 \rangle$  dislocation with  $[-110]$  Burgers vector at 7 nm cutting distance  
200 appears to dissociate to a  $1/3\langle 111 \rangle$  dislocation with  $[11-2]$  Burgers vector. This  
201 phenomenon suggests the shuffle set dislocations could transit to glide set dislocations  
202 under large shear stress caused by the scratching tool [24]. The occurrence of the dual  
203 slip mechanisms was seen an important factor driving plasticity in poly GaAs in sharp  
204 contrast to a single GaAs.





205

206 **Fig. 6.** Variation in the extent of dislocation segments and dislocations images with cutting distance.

207

208 An important physical quantity, dislocation density, was employed to describe the total  
 209 length of dislocation lines contained in a unit volume of polycrystalline GaAs. The  
 210 dislocation density was calculated by Eq. (1) [25].

211

$$\rho = \frac{L}{V} \quad (1)$$

212 where the  $L$  and  $V$  represent the total length of dislocation lines ( $\text{\AA}$ ) and volume of  
 213 workpiece ( $\text{\AA}^3$ ), respectively. Consequently, the evolution of dislocation density as a  
 214 functional of scratching distance is illustrated in Fig. 7.

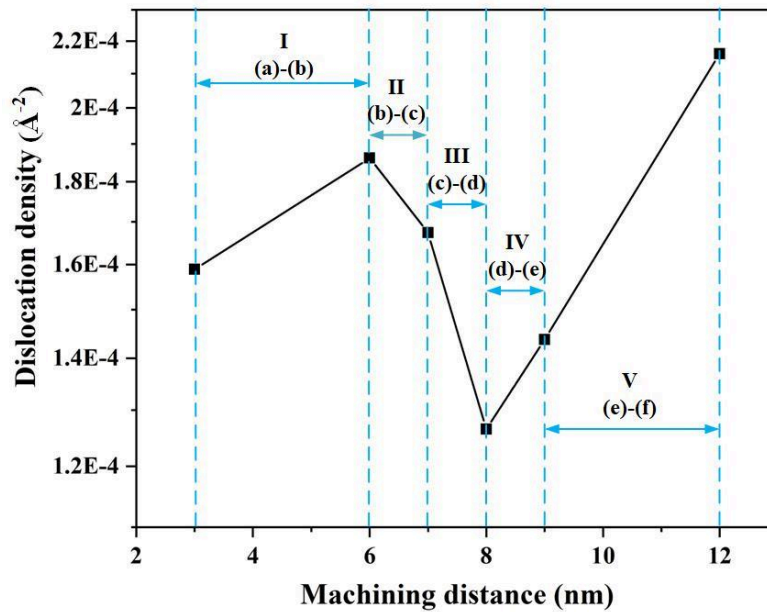


Fig. 7. Evolution of the dislocation density as a function of machining distance.

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218 The dislocation density curve was seen to consist of five stage (I, II, III, IV and V). The

219 dislocation density in the Ist stage was seen to increase which indicated the initiation

220 of dislocation nucleation within the grain boundary. The dislocation density in the IInd

221 and IIIrd stage decreases implied that certain dislocations transform to grain boundaries

222 vis-a-vis disappearing of certain dislocations in a certain grain boundary as shown in

223 Fig. 3 and Fig. 5. The dislocation density of the IV and V stage experienced a significant

224 increase indicating that the diamond tool propagated through the grain boundaries to

225 cause more dislocations and the cycle keeps repeating.

226

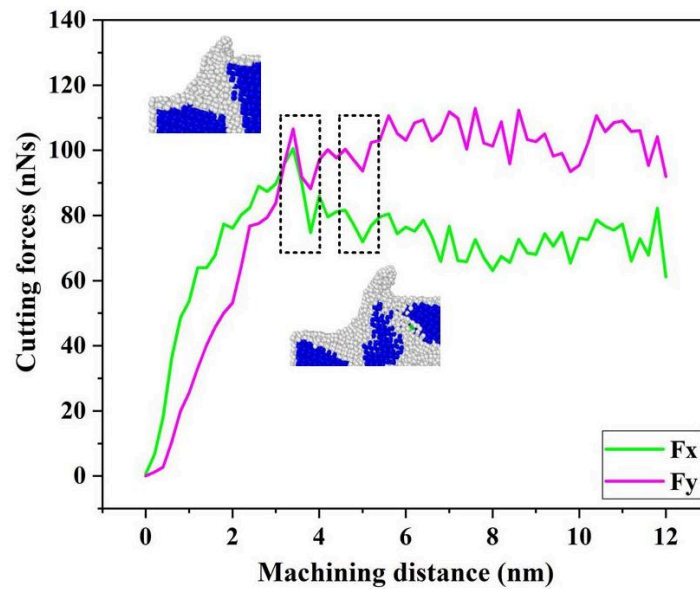
### 227 3.3 Differences in the cutting of single crystal and polycrystalline GaAs

228 During this investigation, additional MD simulations were performed to benchmark the

229 scratch forces namely, the lateral force ( $F_x$ ) and normal force ( $F_y$ ) during cutting of

230 polycrystalline GaAs and single crystal GaAs. Fig 8 shows the evolution of the scratch

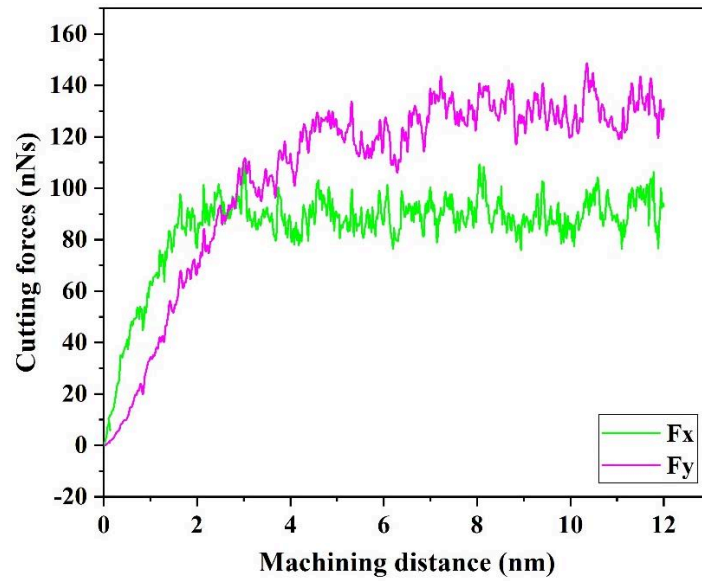
231 forces obtained from the MD simulations while cutting polycrystalline GaAs and single  
232 crystal GaAs substrates. Initially, until the onset of chip formation (unsteady cutting  
233 condition), the lateral force ( $F_x$ ) was seen to be larger than the normal force ( $F_y$ ) and  
234 once the machining achieved a steady-state, then the normal force ( $F_y$ ) becomes larger  
235 than the lateral force. In this study, for the same volume of material removed, the lateral  
236 ( $F_x$ ) and normal force ( $F_y$ ) while cutting polycrystalline GaAs were about 70 nN and  
237 110 nN respectively while the forces during cutting of the single crystal GaAs were of  
238 the order of 90 nN and 130 nN, respectively.



239

240

(a) Scratch forces during cutting of a polycrystalline GaAs



(b) Scratch forces during cutting of a single crystal GaAs

241

242

243 **Fig. 8.** Evolution of cutting forces i.e. lateral ( $F_x$ ) and normal force ( $F_y$ ) at a cutting velocity of 200 m/s

244

and at depth of cut of 2 nm.

245

246 Furthermore, by comparing Fig. 8(a) and Fig. 8(b), it may be seen that the lateral ( $F_x$ )

247 and normal force ( $F_y$ ) smoothly undulated from crests to troughs during cutting of

248 polycrystalline GaAs. The reason for this is that the cutting force drops as the grains

249 started to slide along an easy slip direction and when the grain boundary paved the way

250 for the plastic deformation causing the cutting energy to be mainly concentrated in the

251 grain boundaries. Beyond a certain threshold, the grain boundary collapses releasing a

252 burst of deformation energy which leads to wave troughs of the cutting force.

253 Additional calculations of the specific cutting energy and friction coefficient ( $F_x/F_y$ )

254 were also made. The specific cutting energy is defined as the work done by the tool in

255 removing the unit volume of material and it can be calculated as [26].

$$256 \text{ Specific cutting energy} = \frac{R}{b \times t} \quad (2)$$

257 where  $R$  refers to the resultant force  $\sqrt{F_x^2 + F_y^2}$  while  $b$  and  $t$  represents the width  
 258 of cut and depth of cut, respectively.

259 As shown in Table 2, the resultant cutting force, specific cutting energy and kinetic  
 260 coefficient of friction values for cutting polycrystalline substrate were seen to be lower  
 261 in magnitude compared to cutting single crystal GaAs.

262 **Table 2:** Comparison of cutting results for single crystal GaAs and polycrystalline GaAs

Workpiece	$F_x$ (nN)	$F_y$ (nN)	$F_r$ (nN)	Specific cutting energy (GPa)	Friction coefficient
Single crystal GaAs	91.56	127.35	156.85	27.46	0.719
Polycrystalline GaAs	70.21	103.40	124.98	21.88	0.679

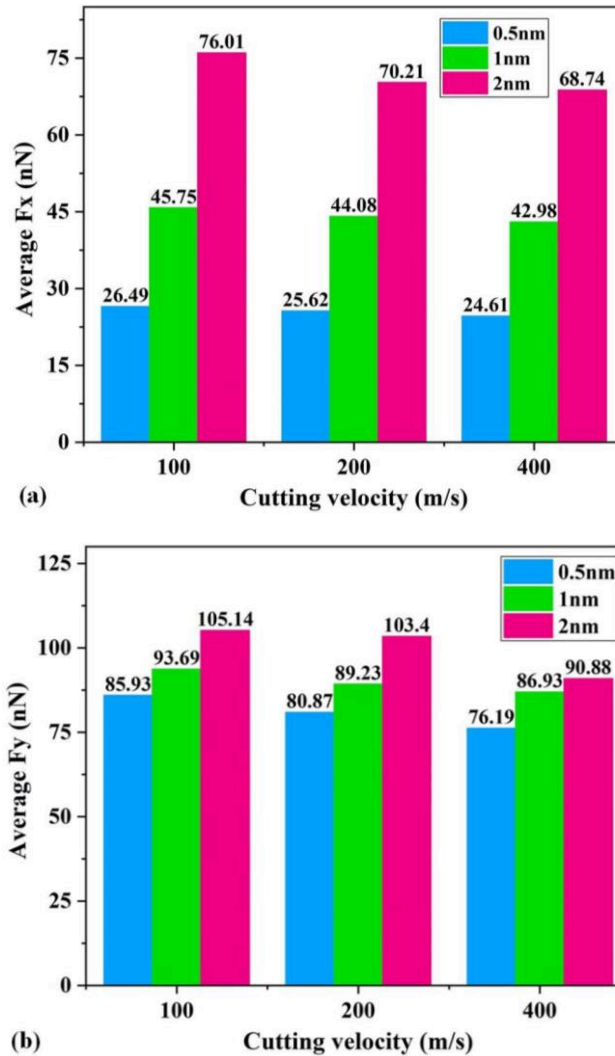
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264 The machining force results indicated that the polycrystalline GaAs was more  
 265 machinable than the single crystal GaAs. This is due to the presence of grain boundaries  
 266 which eases the ductile deformation of a polycrystalline substrate.

267

### 268 *3.4 Influence of cutting depth and cutting speed*

269 In this section, the influence of cutting depth and cutting speed on the cutting forces,  
 270 sub-surface damage depth and the cutting temperature are reported. As shown in Fig. 9,  
 271 both lateral ( $F_x$ ) and normal forces ( $F_y$ ) during cutting of the polycrystalline GaAs  
 272 decreased with the increase of cutting speed or decreasing depth of cut. It was further  
 273 observed that the normal force ( $F_y$ ) continues to be higher than the lateral force ( $F_x$ ) in  
 274 all cases of scratching.



275

276

277 **Fig. 9.** The average value of the lateral ( $F_x$ ) and normal forces ( $F_y$ ) under different cutting velocities

278 and depth of cut in cutting of polycrystalline GaAs.

279

280 Next, the sub-surface damage depth during cutting of polycrystalline GaAs was

281 estimated as a function of different speeds and depth of cut which is shown in figure

282 10. It was seen that the damage depth reduces with the increasing cutting speed which

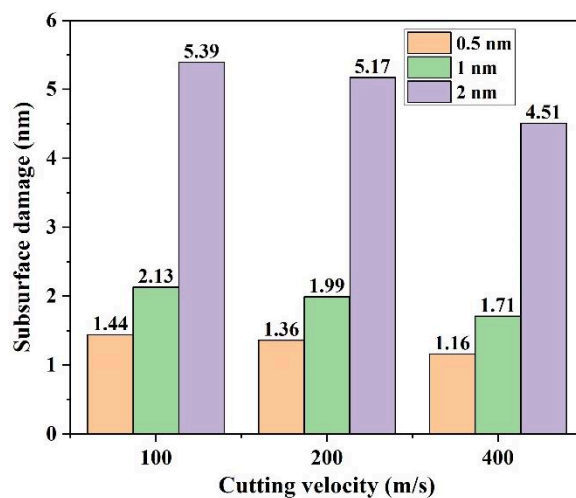
283 indicates that high strain rate applied during cutting decreases the sub-surface damage.

284 A maximum sub-surface damage reduction of 16.32% could be achieved while cutting

285 at 400 m/s at a depth of cut of 2 nm in comparison to cutting at 100 m/s at the same



286 depth of cut.



287

288

**Fig. 10.** Sub-surface damage depth at different cutting velocities and depth of cut

289

Finally, the temperature variation as a function of depth of cut and cutting speed was

290

estimated and shown in figure 11. Higher speed of cutting and higher depths of cutting

291

were both seen to accompany an increase in the cutting temperature in the plastic zone.

292

The combined information of the temperature and stresses acting in the cutting zone

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could be used as a vital information to predict the microstructural changes in the cutting

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zone and we shall expand on this aspect in our future work.

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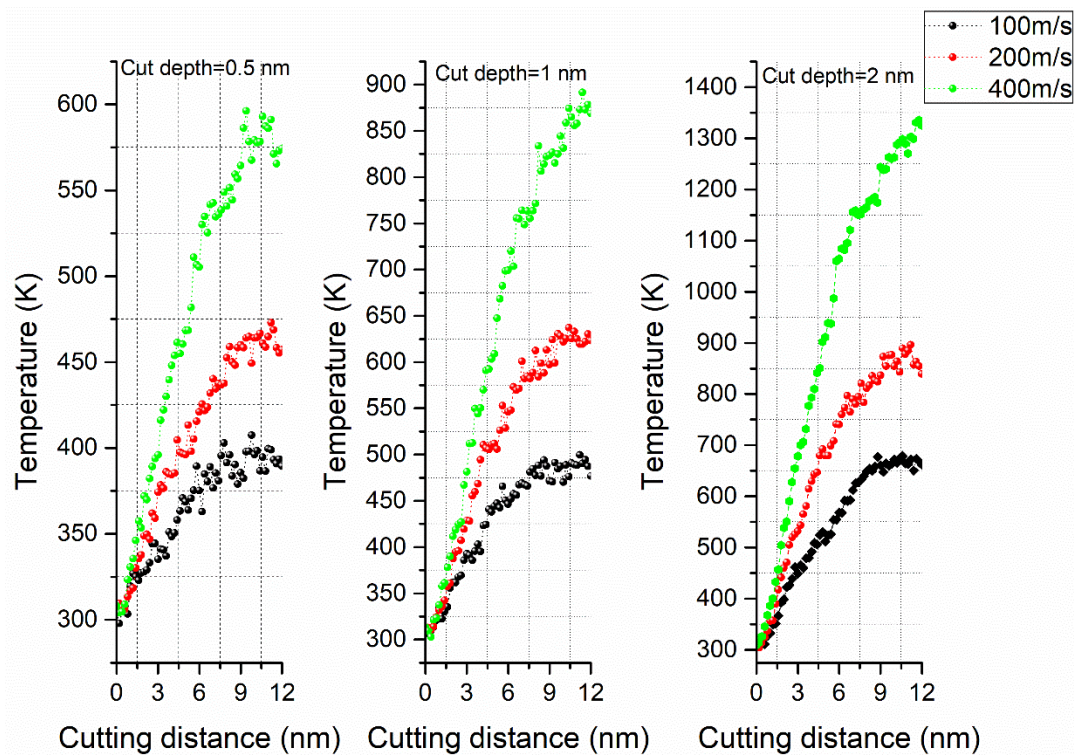


Fig. 11. Peak temperature variation at various scratch speeds and depth of cuts

## 4 Conclusions

In this work, the deformation mechanism of polycrystalline GaAs during nanoscratching was investigated by the MD simulations and benchmarked to single crystal GaAs. During the simulations, the scratch depth, speed of scratching (thus the applied strain rate) and microstructure of the workpiece (polycrystalline vs single crystal GaAs) were varied and output parameters such as the scratch forces (and specific cutting energy), kinetic coefficient of friction, cutting temperature, sub-surface damage and dislocation structures were extracted and analysed. In light of these extracted parameters and the analysis performed, the following conclusions can be drawn:

1. The presence of grain boundaries eases the deformation of the polycrystalline GaAs as opposed to single crystal GaAs. It was discovered that the grain boundaries can become the sites of dislocation nucleation and thus become the

311 weak links in a polycrystal as opposed to a single crystal which has no such  
312 weaker links. The ease of plastic deformation of the grain boundaries compared  
313 to the individual grains makes polycrystals more easily deformed than the single  
314 crystals.

315 2. The cutting forces showed a unique cyclic wave crest to wave troughs transition  
316 while cutting polycrystalline GaAs in contrast to the cutting of the single crystal  
317 GaAs. This was attributable to the periodic arrest of the dislocations in the grain  
318 boundaries followed by collapsed grain boundaries as a result of the continuous  
319 tool penetration.

320 3. The friction coefficient and the specific cutting energy were found to be higher  
321 for scratching single crystal GaAs than for polycrystalline GaAs and also the  
322 normal scratch force achieves a higher magnitude over the lateral scratch force  
323 once the scratching has achieved a steady state.

324 4. Scratch forces and the sub-surface damage were observed to reduce with an  
325 increase in the scratch velocity and to increase with the increasing depth of  
326 scratch. However, the cutting temperature increases with the increase in scratch  
327 speed and the scratch depth.

328 5. Much like the typical diamond cubic lattice structures, the  $\frac{1}{2}\langle 110 \rangle$  was found  
329 to be the main dislocation responsible for plasticity in GaAs which splits into  
330 Shockley partials connected by an Internal Stacking Fault (ISF) leading to  
331 dissociation of the parent dislocation in  $\frac{1}{6}\langle 121 \rangle$  and  $\frac{1}{6}\langle 211 \rangle$  type  
332 dislocations.

333

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348

## 349 **Data statement**

350 All data underpinning this publication are openly available from the University of  
351 Strathclyde Knowledge Base at <https://doi.org/10.15129/ed05ea22-ab4c-4dd7-af36-4dfb91bd1cef>.

353

354 **Conflict of Interest:** The authors declare that they have no conflict of interest.

355

356 **References**

- 357 [1] H. J. Ahn, W. Il Chang, S. M. Kim, B. J. Park, J. M. Yook, and Y. S. Eo, “28  
358 GHz GaAs pHEMT MMICs and RF front-end module for 5G communication  
359 systems,” *Microw. Opt. Technol. Lett.*, vol. 61, no. 4, pp. 878–882, 2019.
- 360 [2] J. H. Epple, K. L. Chang, C. F. Xu, G. W. Pickrell, K. Y. Cheng, and K. C.  
361 Hsieh, “Formation of highly conductive polycrystalline GaAs from annealed  
362 amorphous (Ga,As),” *J. Appl. Phys.*, vol. 93, no. 9, pp. 5331–5336, 2003.
- 363 [3] M. K. Sharma and D. P. Joshi, “Electrical conduction model for polycrystalline  
364 GaAs films,” *J. Appl. Phys.*, vol. 102, no. 3, pp. 1–8, 2007.
- 365 [4] M. Imaizumi *et al.*, “Low-temperature growth of GaAs polycrystalline films on  
366 glass substrates for space solar cell application,” *J. Cryst. Growth*, vol. 221, no.  
367 1–4, pp. 688–692, 2000.
- 368 [5] J. C. Bourgoin, “Polycrystalline GaAs for large area imaging detectors,” *Nucl.*  
369 *Instruments Methods Phys. Res. Sect. A Accel. Spectrometers, Detect. Assoc.*  
370 *Equip.*, vol. 466, no. 1, pp. 9–13, 2001.
- 371 [6] J. D. Song, W. J. Choi, J. I. Lee, J. M. Kim, K. S. Chang, and Y. T. Lee,  
372 “Optical and structural properties of InGaAs/InP double quantum wells grown  
373 by molecular beam epitaxy with polycrystalline GaAs and GaP decomposition  
374 sources,” *Phys. E Low-Dimensional Syst. Nanostructures*, vol. 32, no. 1-2  
375 SPEC. ISS., pp. 234–236, 2006.
- 376 [7] S. Z. Chavoshi, S. Xu, and S. Goel, “Addressing the discrepancy of finding the  
377 equilibrium melting point of silicon using molecular dynamics simulations,”

- 378 *Proc. R. Soc. A Math. Phys. Eng. Sci.*, vol. 473, no. 2202, pp. 1–9, 2017.
- 379 [8] S. Goel, N. Haque Faisal, X. Luo, J. Yan, and A. Agrawal, “Nanoindentation of  
380 polysilicon and single crystal silicon: Molecular dynamics simulation and  
381 experimental validation,” *J. Phys. D. Appl. Phys.*, vol. 47, no. 27, 2014.
- 382 [9] S. Goel, J. Yan, X. Luo, and A. Agrawal, “Incipient plasticity in 4H-SiC during  
383 quasistatic nanoindentation,” *J. Mech. Behav. Biomed. Mater.*, vol. 34, pp.  
384 330–337, 2014.
- 385 [10] S. Goel *et al.*, “Horizons of modern molecular dynamics simulation in  
386 digitalized solid freeform fabrication with advanced materials,” *Mater. Today*  
387 *Chem.*, vol. 18, p. 100356, 2020.
- 388 [11] P. Hirel, “Atomsk: A tool for manipulating and converting atomic data files,”  
389 *Comput. Phys. Commun.*, vol. 197, pp. 212–219, 2015.
- 390 [12] G. Voronoi, “Nouvelles applications des paramètres continus à la théorie des  
391 formes quadratiques. Deuxième mémoire. Recherches sur les paralléloèdres  
392 primitifs,” *J. für die reine und Angew. Math.*, vol. 1908, no. 134, pp. 198–208,  
393 2009.
- 394 [13] G. Lejeune Dirichlet, “Über die Reduction der positiven quadratischen Formen  
395 mit drei unbestimmten ganzen Zahlen.,” *J. für die reine und Angew. Math.*, vol.  
396 40, pp. 209–227, 1850.
- 397 [14] S. Nose, “A unified formulation of the constant temperature molecular-  
398 dynamics methods,” *J. Chem. Phys.*, vol. 81, pp. 511–519, 1984.
- 399 [15] S. J. Plimpton, “Fast parallel algorithms for short range molecular dynamics,”



- 400 *J. Comput. Phys.*, vol. 117, pp. 1–19, 1995.
- 401 [16] D. T. Infield *et al.*, “Main-chain mutagenesis reveals intrahelical coupling in an  
402 ion channel voltage-sensor,” *Nat. Commun.*, vol. 9, no. 1, pp. 1–10, 2018.
- 403 [17] A. Stukowski, “Visualization and analysis of atomistic simulation data with  
404 OVITO-the Open Visualization Tool,” *Model. Simul. Mater. Sci. Eng.*, vol. 18,  
405 no. 1, 2010.
- 406 [18] P. Erhart and K. Albe, “Analytical potential for atomistic simulations of  
407 silicon, carbon, and silicon carbide,” *Phys. Rev. B - Condens. Matter Mater.*  
408 *Phys.*, vol. 71, no. 3, pp. 1–14, 2005.
- 409 [19] K. Albe, K. Nordlund, J. Nord, and A. Kuronen, “Modeling of compound  
410 semiconductors: Analytical bond-order potential for Ga, As, and GaAs,” *Phys.*  
411 *Rev. B - Condens. Matter Mater. Phys.*, vol. 66, no. 3, pp. 352051–3520514,  
412 2002.
- 413 [20] J. F. Ziegler, M. D. Ziegler, and J. P. Biersack, “SRIM - The stopping and  
414 range of ions in matter (2010),” *Nucl. Instruments Methods Phys. Res. Sect. B*  
415 *Beam Interact. with Mater. Atoms*, vol. 268, no. 11–12, pp. 1818–1823, 2010.
- 416 [21] E. Maras, O. Trushin, A. Stukowski, T. Ala-Nissila, and H. Jónsson, “Global  
417 transition path search for dislocation formation in Ge on Si(001),” *Comput.*  
418 *Phys. Commun.*, vol. 205, pp. 13–21, 2016.
- 419 [22] S. Goel and A. Stukowski, “Comment on ‘incipient plasticity of diamond  
420 during nanoindentation’ by C. Xu, C. Liu and H. Wang, : RSC Advances, 2017,  
421 7, 36093,” *RSC Adv.*, vol. 8, no. 10, pp. 5136–5137, 2018.

- 422 [23] S. Goel, X. Luo, P. Comley, R. L. Reuben, and A. Cox, “Brittle-ductile  
423 transition during diamond turning of single crystal silicon carbide,” *Int. J.*  
424 *Mach. Tools Manuf.*, vol. 65, pp. 15–21, 2013.
- 425 [24] Z. Li and R. C. Picu, “Shuffle-glide dislocation transformation in Si,” *J. Appl.*  
426 *Phys.*, vol. 113, no. 8, pp. 1–7, 2013.
- 427 [25] S. H. He, B. B. He, K. Y. Zhu, and M. X. Huang, “Evolution of dislocation  
428 density in bainitic steel: Modeling and experiments,” *Acta Mater.*, vol. 149, pp.  
429 46–56, 2018.
- 430 [26] S. Goel, “The current understanding on the diamond machining of silicon  
431 carbide,” *J. Phys. D. Appl. Phys.*, vol. 47, no. 24, 2014.

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# Origins of ductile plasticity in a polycrystalline gallium arsenide during scratching: MD simulation study

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