Impact dynamics of complex composites modeling including interface between phases
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NUMERICAL MODEL OF METAL-CERAMIC COMPOSITE WITH INTERPHASE PROPERTIES

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ABSTRACT

Multiphase metal matrix composites are used in modern industries like energy, aerospace, and automotive. The materials are used in severe loading conditions like impact loads or thermal shocks. The presentation concerns a data-driven model of an interpenetrated composite. The geometry of the material phases is obtained using CT scanning. Further details, namely, the distribution of voids and inclusions are found with the scanning as well. Based on CT scans the 3D finite element and peridynamics models are derived from. Former analyses [1, 2] showed the importance of the existence of an interface zone in multiphase composites. In the current presentation, the diffusion-based mechanism of forming the interphase zone is shown. A constitutive law evaluated in [3] is considered. The constitutive law for the cohesive zone was obtained using molecular dynamics simulations. The effects of the MD-based law on mesoscale samples are presented.

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Calculations: PL-GRID National Facilities: CYFRONET, Krakow, ICM at the University of Warsaw, TASK, Gdansk, Poland, and LUMI in Kajaani, Finland.

References:

[1] Felten, F., Schneider, G., and Sadowski T. Estimation of R-curve in WC/Co cermet by CT test. Int. J. Refract. Hard. Met., Vol. 26, pp. 55-60, 2008.
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Introductory statement

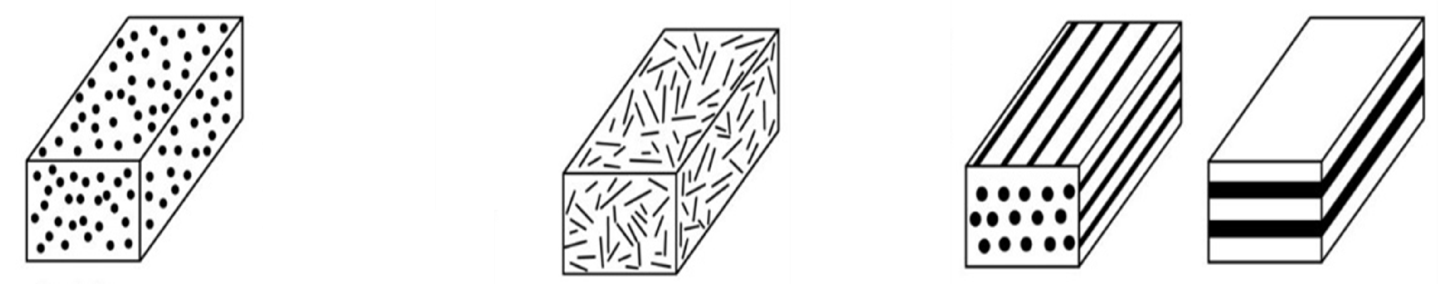
Metal Matrix Composites (MMCs) are widely used in many strategic industrial sectors, such as defense, aerospace, nuclear power plants, spaespace exploration, being the main source of technological progress in the others, for example machining. This rapid development could occur mainly due to their highly desired characteristics, primarily good resistance to transient loadings. Thus, dynamic mechanical testing can be regarded as the design criterion for this kind of materials.

Matrix:
- Aluminum
- Titanium
- Magnesium

Reinforcement:
- Alumina
- Silicon carbide
- Boron carbide

Metal matrix composites (MMCs)

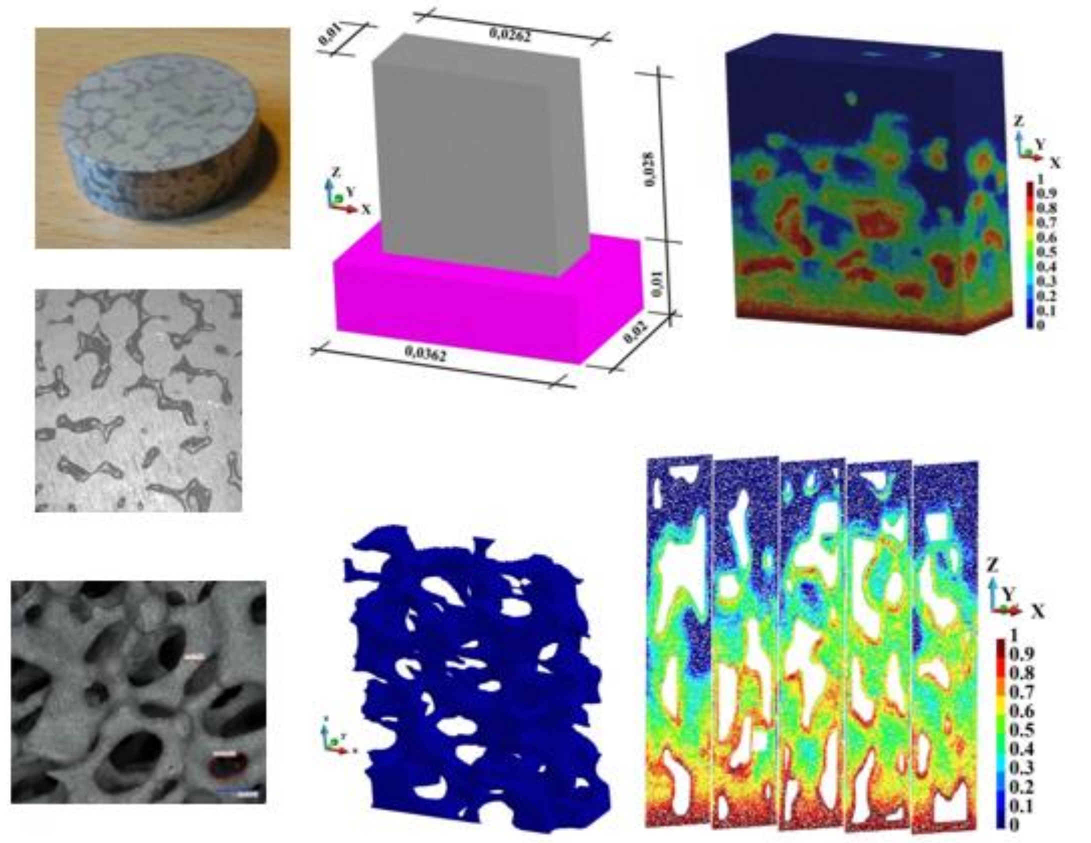
Particles reinforced MMCs | **Short fibers or whiskers reinforced MMCs** | **Continues fibers or sheet reinforced MMCs**



Particles — Short fibers or whiskers — Continues fibers — Sheet laminates

Motivation

Enhancement of the role of interfaces



PERIDIGM (Sandia Lab)
https://github.com/peridigm/peridigm
1) Silling, S.A. Reformulation of elasticity theory for discontinuities and long-range forces. J. Mech. Phys. Solids. 48:175–209, 2000.

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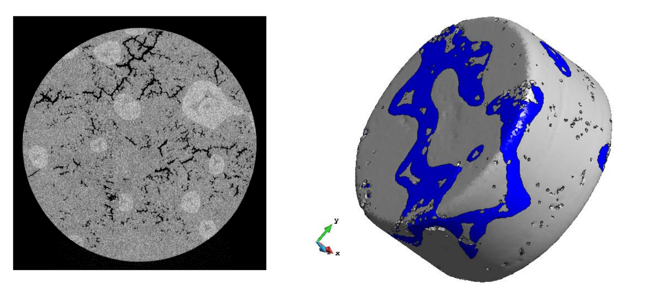
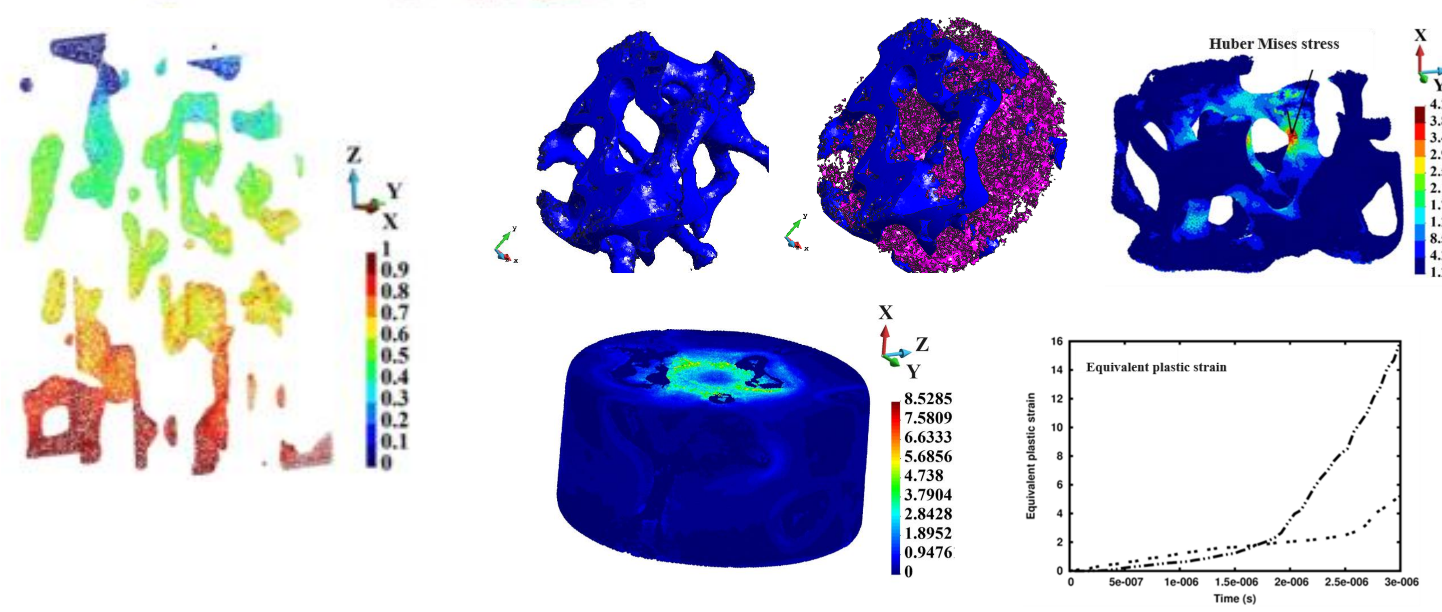
Further CT modeling



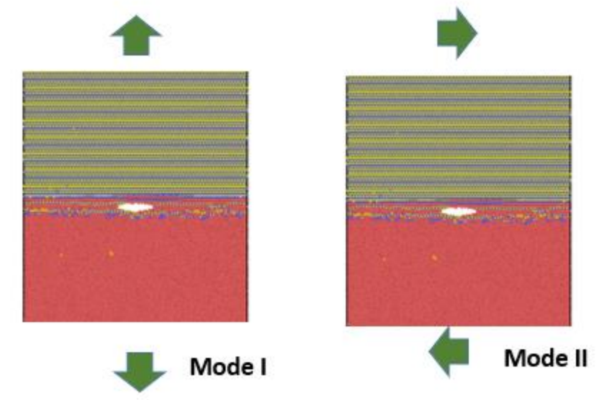
Elastic skeleton with damage condition;
Elastic Plastic with isotropic hardening – the filler



Modelling

Objective — **SiC/Al interface**

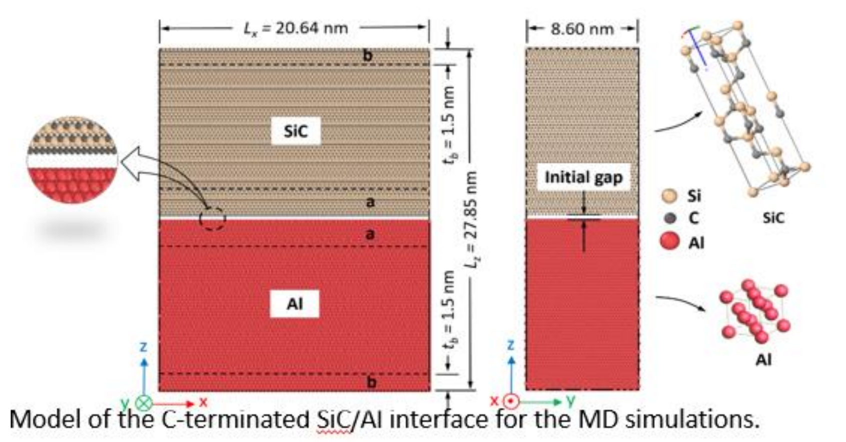
Interdiffusion at the interface → Fuzzy interface → Cohesive zone model → Modes I and II fracture → Interface characteristics



https://www.lammps.org/#gsc.tab=0

Thompson, P, Aktulga, HM, Berger, R, Bolintineanu, DS, Brown,WM, Crozier,PS, in 't Veld, PJ, . Kohlmeyer,A, Moore, SG, Nguyen, TD, Shan, R, Stevens,,MJ, Tranchida, J, Trott, C, Plimpton, SJ, LAMMPS - a flexible simulation tool for particle-based materials modeling at the atomic, meso, and continuum scales. Comp Phys Comm, 271, 10817, 2022.

Simulation model



Model of the C-terminated SiC/Al interface for the MD simulations.

fcc Al
$a = b = c = 4.0495$

Hexagonal SiC (6H-SiC)
$a = b = 3.081$ Å
$c = 15.12$ Å
$\alpha = \beta = 90°, \gamma = 120°$
$(0001)[2\bar{1}\bar{1}0]_{\alpha\text{-SiC}} \| (111)[110]_{Al}$

Cubic SiC (3C-SiC)
$a = b = c = 4.348$ Å
$(111)[01\bar{1}]_{\beta\text{-SiC}} \| (111)[01\bar{1}]_{Al}$

The models used 350,000 atoms, up to 1920 cpus, 39 hours wall clock

Potential functions

Al interactions: The embedded atom method (EAM) potential [1]

$$E_{tot} = \frac{1}{2}\sum_{ij} V(r_{ij}) + \sum_i F(\bar{\rho}_i) \qquad \bar{\rho}_i = \sum_{j \neq i} \rho(r_{ij})$$

Si-C interactions: The Tersoff potential [2]

$$V_{ij} = f_C(r_{ij})\left[f_R(r_{ij}) + b_{ij} f_A(r_{ij})\right]$$

Cut-off potential — Repulsive potential — Attractive potential

Al-Si and Al-C interactions: The Morse potential [3]

System	Parameters	Morse potential
Al-Si	D_0 (eV)	0.4824
	α (1/Å)	1.322
	r_0 (Å)	2.92

System	Parameters	Morse potential
Al-C	D_0 (eV)	0.4691
	α (1/Å)	1.738
	r_0 (Å)	2.246

[1] Y. Mishin, D. Farkas, M.J. Mehl, D.A. Papaconstantopoulos, Physical Rev. B, 59 (1999) 3393-3407.
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[3] H. Zhao, N. Chen, *Inverse Problems* **2008**, *24*, 035019.

Validation of potential functions

$$C_{ij} = \partial\sigma_{ij} / \partial\varepsilon_{ij}$$

Elastic constants — Stress components — Strain components

The elastic constants obtained by the present MD simulations and comparison with those obtained by other investigators.

Material	Method	C_{11} (GPa)	C_{12} (GPa)	C_{44} (GPa)	K (GPa)	E (GPa)	G (GPa)	ν
Al	Present[a]	107.03	61.06	31.05	76.38	62.67	22.99	0.363
	Present[b]	105.09	59.46	30.66	74.67	62.12	22.82	0.361
	MD[c]	107.21	60.60	32.88	76.14	63.44	23.31	0.361
	Experiment[d]	107.3	60.08	28.3	75.7	63.83	23.48	0.359
3C-SiC	Present	383.78	144.41	239.75	224.20	304.81	119.68	0.273
	MD[e]	390.1	142.7	191.0	225.1	313.6	123.7	0.268
	Experiment[f]	390	142	256	225	314.2	124	0.267

[a] The EAM potential. Y. Mishin, D. Farkas, M.J. Mehl, D.A. Papaconstantopoulos, Physical Rev. B, 59 (1999) 3393-3407.
[b] The EAM potential. M.I. Mendelev, M.J. Kramer, C.A. Becker, M. Asta, Philosophical Magazine, 88 (2008) 1723-1750.
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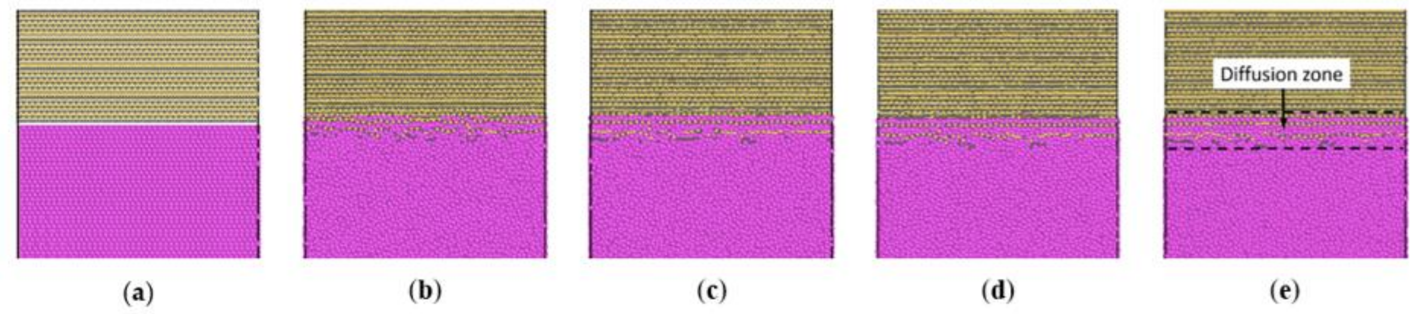
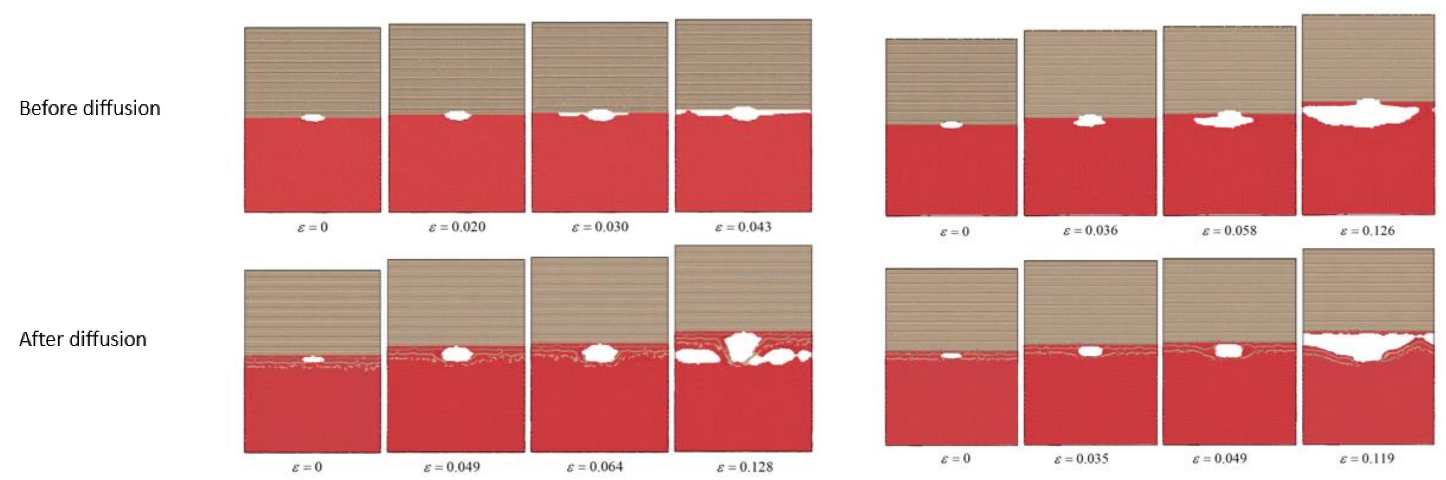
[e] P. Vashishta, R.K. Kalia, A. Nakano, J.P. Rino, J. Appl. Phy., 101 (2007).
[f] D.W. Feldman, J.H. Parker, W.J. Choyke, L. Patrick, Phys. Rev., 173 (1968) 787-793.

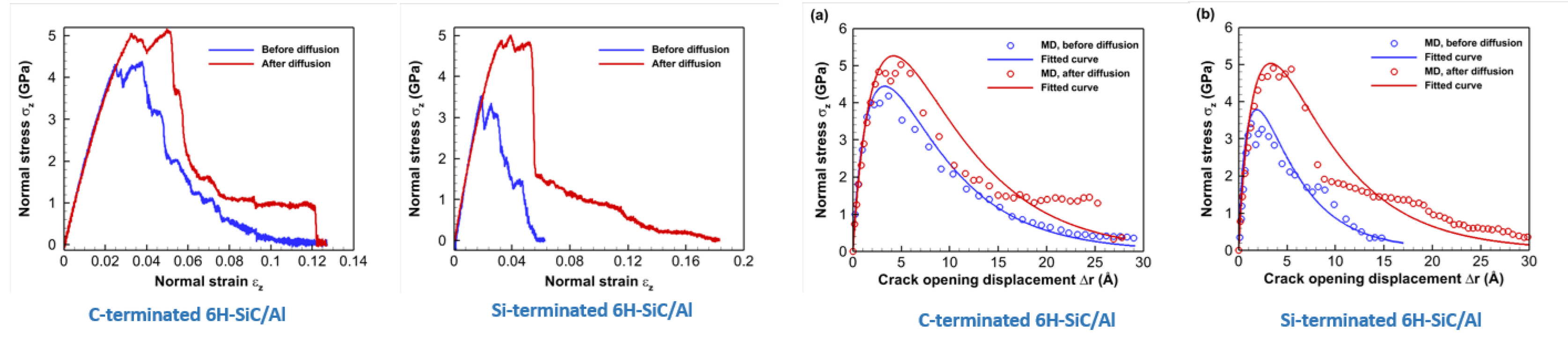
Interdiffusion at 2000 K



Cross-sectional views of the atomic configurations of C-terminated 6H-SiC/Al interface. **(a)** Atomic structure at 300 K before relaxation and the configuration after maintaining the system at 2000 K for **(b)** 0 ns, **(c)** 2 ns, **(d)** 4 ns and **(e)** 6 ns.



Si-terminated 6H-SiC/Al under pure tensile loading (mode I). — C-terminated 6H-SiC/Al under pure tensile loading (mode I).



Stress-strain relation for SiC/Al composite under tensile loading for both cases before and after heat treatment.

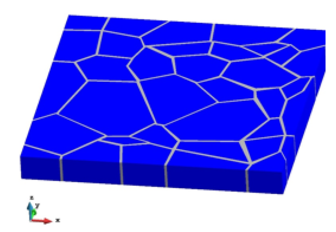
Traction-separation relation for SiC/Al composite under tensile loading for both cases before and after heat treatment.

The elastic modulus, maximum tensile stress, toughness, and work of complete separation of mode I failure tests.

Composite material	Annealing condition	E (GPa)	σ_{max} (GPa)	Toughness (10^9 J/m³)	Work of se (J/m²)
C-terminated 6H-SiC/Al	Before diffusion	159.7	4.39	0.174	4.81
	After diffusion	163.5	5.17	0.231	6.41
Si-terminated 6H-SiC/Al	Before diffusion	162.9	3.55	0.052	2.49
	After diffusion	164.7	5.02	0.217	5.59
C-terminated 3C-SiC/Al	Before diffusion	165.5	4.40	0.164	4.50
	After diffusion	167.4	5.40	0.183	5.71
Si-terminated 3C-SiC/Al	Before diffusion	163.7	3.57	0.071	3.17
	After diffusion	166.0	5.21	0.232	6.21

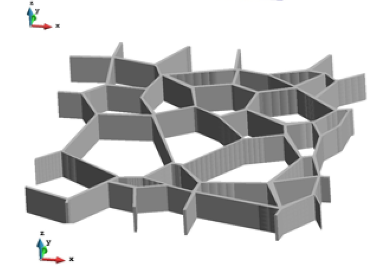
The shear modulus and maximum shear stress of mode II failure tests.

Composite material	Annealing condition	G (GPa)	τ_{max} (GPa)
C-terminated 6H-SiC/Al	Before diffusion	36.9	1.71
	After diffusion	36.5	1.80
Si-terminated 6H-SiC/Al	Before diffusion	39.2	1.12
	After diffusion	35.2	1.82
C-terminated 3C-SiC/Al	Before diffusion	39.8	1.72
	After diffusion	32.2	1.60
Si-terminated 3C-SiC/Al	Before diffusion	33.1	1.39
	After diffusion	30.7	1.65

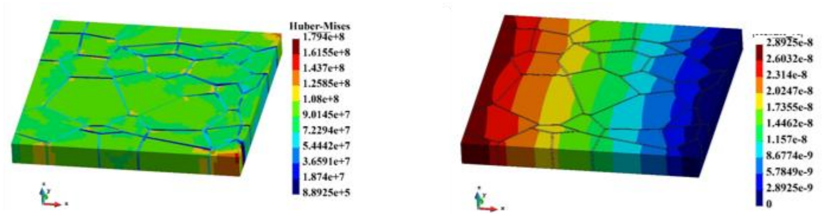


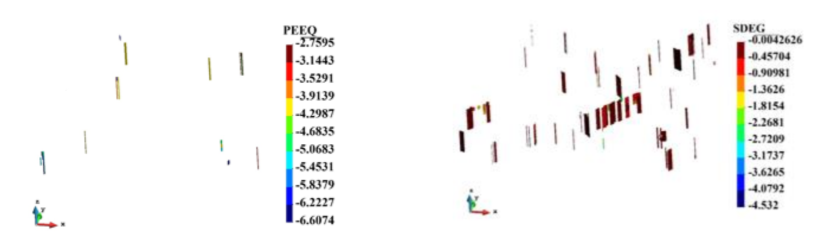
SiC, grain – Young's modulus 4.09E+11Pa,
Poisson's ratio 0.16
AlSi12, interface – Young's modulus 67.0e+09 Pa
Poisson's ratio 0.35
Yield limit 100.0E+06 Pa

Interface: E – 159.7E+09 Pa, failure at 0.08,
separation energy 4.81 J/m2



Loading – pressure (tension), 80.0E+06 Pa





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National Science Centre Poland — University of Stuttgart