MODA for void growth modelling

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Disclaimer

Chapter 1 MODA Tables

The AddMorePower consortium is dedicated to developing characterization and modelling methods that can meet the unique needs of upcoming power semiconductor technology generations. To achieve effective and efficient research and innovation, a seamless interoperation between materials characterization, materials modelling, and data science is required. This goal can only be accomplished through the use of FAIR and open data practices.

AddMorePower employs the CHADA and MODA methodologies to achieve FAIR data management. These systematic description and documentation methods are used for materials characterization data and materials modelling data, respectively. They are based on a common terminology, concepts and relationships defined by the community, providing a holistic approach to combine data from various materials characterization and modelling techniques, which allows analysing and modelling of complex structures.

In this document the MODA for void growth modelling simulated in the project AddMorePower is presented. The MODA is based on the template released by emmc.eu in May 2021 [2] and the common terminology defined in the CEN Workshop Agreement 17284 [1].

OVERVIEW of the SIMULATION			
1	**USER CASE**	*The metallization plate of power semiconductors plays an important role in the thermal management. During service, it might lose its structural integrity due to void formation and growth.*	
2	**CHAIN OF MODELS**	**MODEL 1**	*The mechanical continuum model for static equilibrium is coupled to a crystal plasticity model for plastic deformation in the matrix and a void growth model to study void growth at a grain boundary.*
3	**PUBLICATION PEER-REVIEWING THE DATA**	*This simulation has not been published yet*	
4	**ACCESS CONDITIONS**	*DAMASK (https://damask.mpie.de) has been used. DAMASK is free and open source software according to AGPL v3 [4].*	
5	**WORKFLOW AND ITS RATIONALE**	*The aim of this workflow is to investigate the void growth rate in dependency of the internal pressure of the void at a grain boundary. To correctly include the anisotropic plastic flow of metals, a crystal plasticity model is used for the matrix. In the absence of a model for pressure increase, the void is modelled as an elastic material with volume expansion due to temperature increase.*	

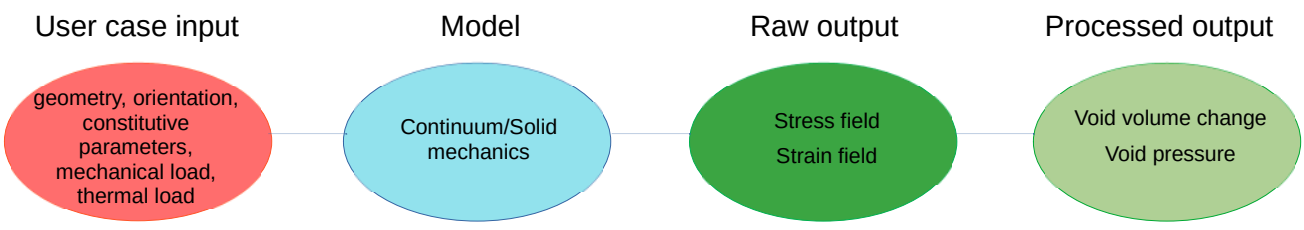
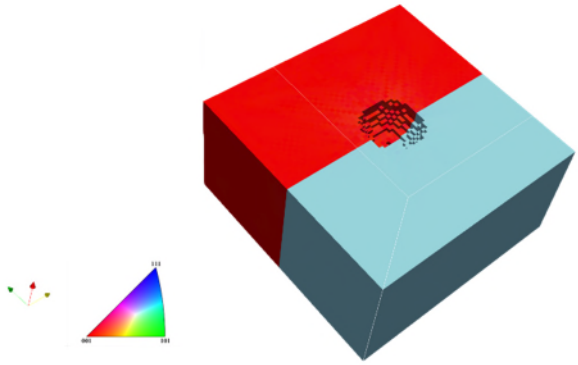


Figure 1: Void growth modelling workflow based on MODA workflow template [3]

1.1 MODA – Physics-based Model

MODEL 1

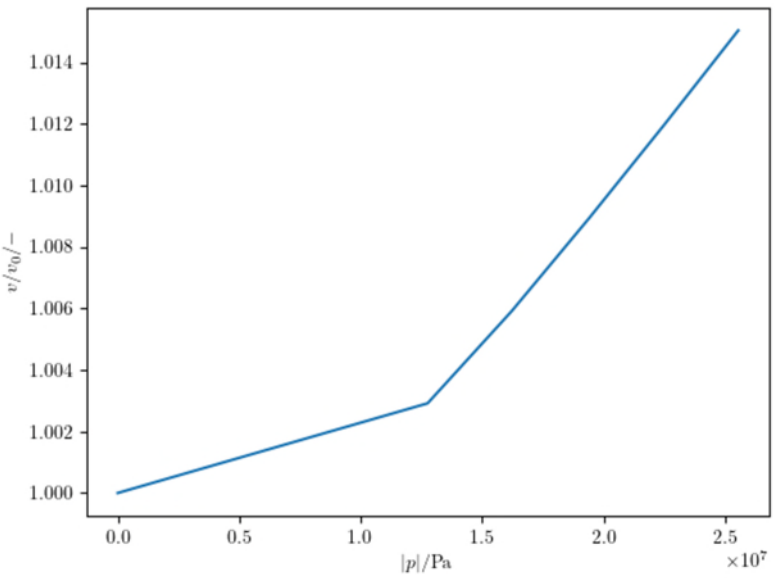
Void growth at grain boundary

1	ASPECT OF THE USER CASE/SYSTEM TO BE SIMULATED	
1.1	ASPECT OF THE USER CASE TO BE SIMULATED	*Prediction of void growth rate in dependence of the internal pressure.*
1.2	MATERIAL	*Electrochemically deposited thin film polycrystalline copper metallization (<20µm) and organic trace impurities*
1.3	GEOMETRY	*Bicrystal with spherical void. Shown below is a cut along the x-direction, the grain boundary is along the z-direction. Colour code is according to the inverse pole figure (IPF) along the z-direction.* 
1.4	TIME LAPSE	*500s*
1.5	MANUFACTURING PROCESS OR IN-SERVICE CONDITIONS	*The stress on the sides of the volume element is set to 0.0 MPa*
1.6	PUBLICATION ON THIS DATA	*n/a*

2	GENERIC PHYSICS OF THE MODEL EQUATION		
2.0	MODEL TYPE AND NAME	*Continuum model/Solid Mechanics.*	
2.1	MODEL ENTITY	*The entities in this material model are finite volumes/grains.*	
2.2	MODEL PHYSICS/ CHEMISTRY EQUATION PE	**Physical Equation**	*Conservation of linear momentum ("Cauchy's first law of motion"):* div(***P***) = ***0*** *The static mechanical equilibrium is presented in a large strain formulation. A multiplicative decomposition of the deformation gradient **F** is used:* $\boldsymbol{F} = \boldsymbol{F}_e \boldsymbol{F}_i \boldsymbol{F}_p$ *In the matrix,* $\boldsymbol{F}_p$ *evolves according to a crystal plasticity law. In the void, the diagonal components of* $\boldsymbol{F}_i$ *are increased linearly with time.*
		Physical Quantities	***div** : Divergence operator* ***P** : First Piola-Kirchhoff stress tensor* $\boldsymbol{F}_e$ *: Elastic deformation gradient* $\boldsymbol{F}_i$ *: Lattice distorting, inelastic deformation gradient* $\boldsymbol{F}_p$ *: Lattice preserving, inelastic deformation gradient*
2.3	MATERIALS RELATIONS	**Relation**	*Linear **elasticity** (in the void)* - Generalized Hooke's law **S = C : E** - Elastic constants ***Elasto-viscoplasticity** (in the matrix)* *- Plastic velocity gradient (per system* α *= 1 .. N)* $L_p = \Sigma_\alpha \dot{\gamma_\alpha} (s_s^\alpha \otimes n_s^\alpha)$ *- Phenomenological crystal plasticity* *- Shear in a slip system* $\dot{\gamma^\alpha} = \dot{\gamma_0} \left\lvert \frac{\tau^\alpha}{\xi^\alpha} \right\rvert^n sgn(\tau^\alpha)$ *- Deformation resistance* $\dot{\xi} = h_0 \left(1 - \frac{\xi}{\xi_\infty}\right)^a sgn\left(1 - \frac{\xi}{\xi_\infty}\right)$
		Physical quantities/ descriptors for each MR	***C** : fourth-order elasticity tensor (**C** =* C_{ijkl} *, with only three independent components* C_{11}*,* C_{12}*,* C_{44} *for cubic crystals)* ***E**: Green-Lagrange strain tensor: **E** = ½* $\boldsymbol{F}_i^T(\boldsymbol{F}_e^T \boldsymbol{F}_e - \boldsymbol{I})\boldsymbol{F}_p$ *-- **I** is the identity tensor* ***N** : number of slip systems* ***s**, **n** : Unit vectors along the shear direction and shear plane normal* γ *: Shear strain (*γ_0 *: reference shear strain)* τ *: Resolved shear stress* *n : Rate exponent* ***ξ** : Deformation resistance (initial* ξ_0*, saturation* ξ_∞*)* *a : Hardening exponent* ***Other**: crystal orientations*
2.4	SIMULATED INPUT	*n/a*	

3	SOLVER AND COMPUTATIONAL TRANSLATION OF THE SPECIFICATIONS		
3.1	NUMERICAL SOLVER	*Spectral solver using FFT (DAMASK_grid with forward backward difference scheme)*	
3.2	SOFTWARE TOOL	*DAMASK (license AGPL v3)* *https://damask.mpie.de* *https://doi.org/10.1016/j.commatsci.2018.04.030*	
3.3	TIME STEP	*0.2 seconds (50 times steps for a total of 10 simulation seconds)*	
3.4	COMPUTATIONAL REPRESENTATION	PHYSICS EQUATION, MATERIAL RELATIONS, MATERIAL	*The deformation gradient is split into an average part and a fluctuating part. The fluctuating part is adjusted until the resulting stress is in mechanical equilibrium*
3.5	COMPUTATIONAL BOUNDARY CONDITIONS	*The boundary conditions are given in terms of the volume average on a periodic domain*	
3.6	ADDITIONAL SOLVER PARAMETERS	*Derivative approximation: FWBW_Difference* *Field equations are solved using fully implicit time stepping* *Equilibrium of the mechanical stress field is ensured by evaluating the Root Mean Square (RMS) value of the divergence of the stress field*	

1.2 MODA – Post Processing

4	POST PROCESSING	
4.1	THE PROCESSED OUTPUT	*The volume change of the void (v/v_0) is plotted as a function of the absolute pressure (p) in the void.* 
4.2	METHODOLOGIES	*1) First, the Cauchy stress is calculated from the deformation gradient **F** and the second Piola-Kirchhoff stress **S**. Then, the absolute pressure p of the Cauchy stress is calculated.* *2) The determinant of the deformation gradient is calculated to obtain the change in volume in the void v/v_0.* *Both quantities are averaged over the volume of the void. All relations are standard in continuum mechanics.*
4.3	MARGIN OF ERROR	*The post processing is exact.*

Chapter 2 List of Abbreviations

Abbreviation	Translation
AlGaN	Aluminium Gallium Nitride
CMOS	Complementary Metal-Oxide-Semiconductor
DAMASK	Düsseldorf Advanced Material Simulation Kit
EMCC	European Materials Characterization Council
EMMC	European Materials Modelling council
FWBW	Forward backward difference scheme
MODA	Materials Modelling Data
ms	milliseconds

Bibliography

[1] *CWA 17284 – Materials modelling – Terminology, classification and metadata*, October 2018
[2] Emmc.eu, *MODA template*, 2021.
[3] Emmc.eu, *MODA workflow template*, 2021.
[4] DAMASK, DAMASK (https://damask.mpie.de). Free and open source software according to AGPL v3