On the Size of the Representative Volume Element for Isotropic Elastic Polycrystalline Copper

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Abstract. A computational homogenization strategy is developed to determine the number of grains necessary to estimate the effective elastic properties of isotropic polycrystalline copper with a given precision. Finite element simulations of polycrystalline aggregates are presented for both homogeneous and periodic boundary conditions. For different volumes, several realizations are considered. The mean apparent shear modulus and the associated dispersion are estimated as a function of the number of grains. Periodic conditions lead to rapid convergence of the result towards the wanted effective shear modulus. The Representative Volume Element (RVE) size is then related to the evolution of the standard deviation of the apparent shear modulus, via an extension of the notion of integral range A_3. For a precision of 1% and 10 realizations, a minimal RVE size of 445 grains is found. The found value $A_3 = 1.43$ can be compared to the integral range for other microstructures and physical properties.

Key words: representative volume element, homogenization, polycrystal, copper, finite element, integral range.

1 Introduction

Computational homogenization methods are nowadays efficient tools to estimate effective properties of heterogeneous materials. They can take realistic distribution of phases and sophiscated constitutive equations of the constituents into account (Cailletaud et al., 2003). A key-point in such models is the determination of the appropriate size of volume elements of heterogeneous materials to be computed in order to get a precise enough estimation of effective properties. This is related to the long-standing problem of the determination of the size of the Representative Volume Element (RVE) in homogenization theory (Drugan, 1996). It is known that RVE is morphology and property dependent but a well-suited parameter is necessary for quantitative comparisons. Such a parameter was proposed by Kanit et al. (2003).

In the present work, a method is proposed to estimate the size of such a RVE in isotropic linear elastic copper polycrystals. It has three main steps: the choice

Yilong Bai et al. (eds), IUTAM Symposium on Mechanical Behavior and Micro-Mechanics of Nanostructured Materials, 171–180.

of a random model for polycrystalline microstructures containing a finite number of grains, the resolution of boundary value problems on polycrystalline aggregates of increasing sizes and the analysis of the convergence of the calculated apparent properties towards an asymptotic value as a function of the number of grains and of the boundary conditions. The asymptotic value is regarded as the effective property (Sab, 1992). In other words, the objective is to find the minimum number of grains required in a volume element to estimate the effective elastic property with a given accuracy. The size of the RVE for several cubic elastic polycrystals was investigated in 2D by Ren and Zheng (2002) and by Nygårds (2003) using three-dimensional FE simulations and periodic boundary conditions. A relationship between the RVE size and the anisotropy coefficient of each material was identified. Most interestingly, the last author links the notion of representativity of considered material volumes with the decay of the dispersion of calculated apparent properties for increasing grain numbers, as done by Kanit et al. (2003). The present contribution focuses on the dependence of the result on the choice of boundary conditions and on the determination of a statistical parameter quantifying the decrease in scatter with increasing grain numbers and allowing comparisons of RVE sizes for other microstructures and properties.

In the following, vectors are underlined and boldface quantities are second-rank or fourth-rank tensors. The symbol := defines the quantity on the left of the symbol.

2 Computational Homogenization Method

2.1 Generation of Microstructures

Voronoi mosaics are used here as a random model to represent the polycrystalline morphology, as explained in Barbe et al. (2001) and Kanit et al. (2003). For each realization, one given cubic volume V that contains a given number N_g of Voronoi cells is simulated. In the following, n realizations of volume V are considered. The number of cells for each realization of the microstructure obeys a Poisson distribution with given mean value $\bar{N}_g = N$. The mean volume of one Voronoi cell is equal to 1. No unit length is introduced because the models involved in this work cannot account for absolute size effects. As a result, one has $N = V$. This convention is used throughout the work.

A crystal orientation is attributed to each Voronoi cell which is then regarded as an individual grain of the polycrystal. The crystallographic texture is assumed to be random. It is possible to impose a geometrical periodicity constraint at the boundary of the polycrystalline cube, as shown in Figure 1 (see also Kanit et al., 2003). This condition is enforced in the subsequent FE simulations involving periodicity conditions.

2.2 FE Meshing of Microstructures

The so-called multi-phase element technique is used in order to superimpose a regular 3D FE mesh on the Voronoi tessellation point of each element of the mesh.

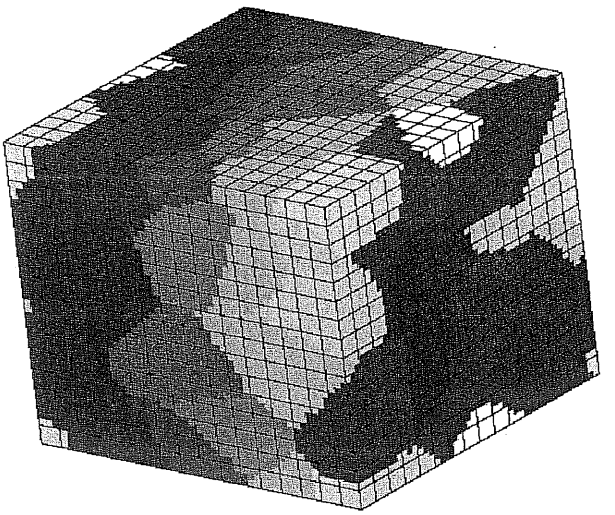

Fig. 1. Regular FE mesh superimposed on a Voronoi mosaic containing 50 grains, using the multiphase element technique.

The crystal orientation of the closest voxel is attributed to every integration point of each element of the mesh. The elements are 20-node quadratic bricks with 27 Gauss points. Figure 1 shows such a mesh made of $16 \times 16 \times 16$ elements. The main drawback of the technique is that one element may contain integration points that belong to several grains. The bias introduced by this meshing technique was investigated in Schmauder (1997), Barbe et al. (2001) and Kanit el al. (2003).

The effect of mesh density, i.e. of the number of elements per grain, was investigated here for elastic polycrystalline copper. FE meshes of a given aggregate made of 50 grains were considered. The convergence of the computed apparent shear modulus μ^{app} was analyzed when the number of mesh elements increases. For each simulation, the geometry of the microstructure is unchanged but the number of degrees of freedom is increased from 5568 to 56355. From these results, a resolution of 16 elements per grain was chosen for the following calculations. The use of finer meshes does not improve the result of more than 1%.

The largest volume computed in this work is a cube with $423 = 74088$ elements, i.e. 937443 degrees of freedom. Such computations are made possible in a reasonable time by using parallel computing. The FE program used in this work implements the subdomain decomposition method FETI (Zset, 1996; Feyel, 1999). The mesh is split into 32 subdomains and the tasks are distributed on a platform of 32 processors (768 MB RAM, 800 MHz). Compatibility and equilibrium at interfaces between subdomains are restored by an iterative procedure. The whole resolution requires 21GB of memory.

2.3 Boundary Conditions and Definition of Apparent Moduli

Three types of boundary conditions to be prescribed on an individual volume element V are considered (Zaoui, 1987):

- *Kinematic uniform boundary conditions* (KUBC): The displacement vector $\underline{u}$ is imposed at all points x belonging to the boundary ∂V according to:

$$\underline{u} = \mathbf{E} \cdot \underline{x} \quad \forall \underline{x} \in \partial V \quad \langle \boldsymbol{\varepsilon} \rangle := \frac{1}{V} \int_V \boldsymbol{\varepsilon} dV = \mathbf{E}, \tag{1}$$

  where E is a given constant symmetrical second-rank tensor. The macroscopic stress tensor $\boldsymbol{\Sigma}$ is then defined as the spatial average of the local stress tensor $\boldsymbol{\sigma}$.
- *Static uniform boundary conditions* (SUBC): The traction vector is prescribed at the boundary ∂V according to:

$$\boldsymbol{\sigma} \cdot \underline{n} = \boldsymbol{\Sigma} \cdot \underline{n} \quad \forall \underline{x} \in \partial V \quad \langle \boldsymbol{\sigma} \rangle := \frac{1}{V} \int_V \boldsymbol{\sigma} dV = \boldsymbol{\Sigma}, \tag{2}$$

  where $\boldsymbol{\Sigma}$ is a given constant symmetrical second-rank tensor. The outer normal to ∂V at x is denoted by n. The macroscopic strain tensor E is then defined as the spatial average of the local strain ε.
- *Periodicity conditions* (PERIODIC): The displacement field over the entire volume V takes the form

$$\underline{u} = \mathbf{E} \cdot \underline{x} + \underline{v} \quad \forall \underline{x} \in \partial V, \tag{3}$$

  where the fluctuation $\underline{v}$ is periodic. $\underline{v}$ (resp. $\boldsymbol{\sigma} \cdot \underline{n}$) takes the same value (resp. opposite value) at two homologous points on opposite sides of V.

The local behaviour at every integration point inside each grain in the simulation is described by the fourth-rank linear elasticity tensor $\mathbf{c}$:

$$\boldsymbol{\sigma}(\underline{x}) = \mathbf{c}(x) : \boldsymbol{\varepsilon}(\underline{x}). \tag{4}$$

No specific behavior is attributed to grain boundaries (Cailetaud et al., 2003). The partial differential equations to be solved using the FE method are the classical stress balance equations without body forces. For a given volume V, and owing to the linearity of the considered boundary value problems, fourth-rank tensors of apparent moduli C_E^{app} and apparent compliance S_Σ^{app} can be defined by the following macroscopic relations:

$$\boldsymbol{\Sigma} = \langle \boldsymbol{\sigma} \rangle = \frac{1}{V} \int_V \boldsymbol{\sigma} dV = \mathbf{C}_E^{\text{app}} : \mathbf{E}, \quad \mathbf{E} = \langle \boldsymbol{\varepsilon} \rangle = \frac{1}{V} \int_V \boldsymbol{\varepsilon} dV = \mathbf{S}_\Sigma^{\text{app}} : \boldsymbol{\Sigma}. \tag{5}$$

The first relation is used for KUBC and PERIODIC problems, the second one for SUBC problems. Note that in general, the tensor S_Σ^{app} cannot be expected to coincide with the inverse of C_E^{app}. However, for sufficiently large volumes V, the apparent moduli do not depend on the type of boundary conditions any longer and coincide with the effective properties of the medium (Sab, 1992):

$$\mathbf{S}_\Sigma^{\text{app}-1} = \mathbf{S}^{\text{eff}-1} = \mathbf{C}^{\text{eff}} = \mathbf{C}_E^{\text{app}}. \tag{6}$$

For intermediate volumes V, the following inequalities, written in the sense of quadratic forms, hold (Huet, 1990):

$$\mathbf{S}_{\Sigma}^{\text{app}-1} \leq \mathbf{C}^{\text{eff}} \leq \mathbf{C}_{E}^{\text{app}}. \tag{7}$$

In the next section, both C_E^{app} and the periodic estimations are checked to remain between the bounds defined by (7).

The following two shear loading conditions E_μ and Σ_μ are used in this work:

$$E_\mu = \begin{bmatrix} 0 & \frac{1}{2} & 0 \\ \frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad \Sigma_\mu = \begin{bmatrix} 0 & \alpha & 0 \\ \alpha & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \quad \text{with } a = 1 \text{ MPa} \tag{8}$$

in the particular Cartesian coordinate frame attached to the cubic volume element. In the case of KUBC and PERIODIC conditions prescribed to a given volume V, one defines the apparent modulus μ_E^{app} by the work of internal forces in the volume V subjected to the loading E_μ:

$$\mu_E^{\text{app}}(V) := \langle \boldsymbol{\sigma} : \boldsymbol{\varepsilon} \rangle = \langle \boldsymbol{\sigma} \rangle : \mathbf{E}_\mu = \frac{1}{V} \int_V \sigma_{12} dV. \tag{9}$$

In the case of SUBC boundary conditions, an apparent shear modulus μ_Σ^{app} is defined as the work of internal forces generated in V by the application of the loading Σ_μ:

$$\frac{a^2}{\mu_E^{\text{app}}}(V) := \langle \boldsymbol{\sigma} : \boldsymbol{\varepsilon} \rangle = \Sigma_\mu : \langle \boldsymbol{\varepsilon} \rangle = \frac{2a}{V} \int_V \varepsilon_{12} dV. \tag{10}$$

These definitions remain formal insofar as the apparent elasticity properties of a given material volume element V are not necessarily isotropic.

3 Determination of Apparent Shear Moduli for Polycrystalline Copper

We now consider the special case of linear elastic copper polycrystals with a uniform distribution of crystal orientations. The cubic elasticity constants of pure copper are taken from Gairola (1981):

$$C_{11} = 168400 \text{ MPa}, \quad C_{12} = 121400 \text{ MPa}, \quad C_{44} = 75390 \text{ MPa}.$$

The corresponding value of the anisotropy coefficient $\alpha = 2C_{44}/(C_{11} - C_{12})$ is 3.2.

Due to the uniform distribution of crystal orientations, the effective medium exhibits an isotropic linear elastic behaviour, described by effective bulk and shear moduli k^{eff} and μ^{eff}. For cubic symmetry, the apparent bulk modulus is not a random variable (Gairola, 1981). It is uniquely determined from the single crystal elasticity constants according to the formula $k^{\text{app}} = k^{\text{eff}} = (C_{11} + 2C_{12})/3 = 137067$ MPa. As a result, the homogenization problem reduces to the estimation of apparent shear properties μ^{app} and *in fine* of the effective shear modulus μ^{eff}.

Table 1. Mean apparent shear modulus, associated dispersion and relative error on the mean as a function of the domain size and of the number of realizations for three different boundary conditions.

	V	n	$\bar{\mu}^{\text{app}}$ (MPa)	$D_\mu(V)$ (MPa)	ε_{rel}
KUBC	25	100	52543	3186	1.2%
KUBC	400	50	50088	836	0.4%
KUBC	1000	25	49787	533	0.4%
KUBC	5000	10	49336	222	0.2%
PERIODIC	25	100	49669	3162	1.2%
PERIODIC	123	50	48886	1400	0.8%
PERIODIC	400	50	48784	811	0.4%
PERIODIC	500	50	48764	778	0.4%
SUBC	25	100	43397	3185	1.4%
SUBC	400	50	47308	823	0.4%
SUBC	1000	25	47566	538	0.4%
SUBC	5000	10	48390	178	0.2%

It is shown in Kanit et al. (2003) that the fourth-rank tensor of apparent moduli $C_E^{\text{app}}(V)$ obtained for a finite domain V containing N_g grains is generally not isotropic. However, its ensemble average $\bar{C}_E^{\text{app}}(V)$, i.e. its mean value over a sufficiently large number of realizations, turns out to be isotropic. This has been checked here for polycrystalline copper aggregates. The shear modulus associated with the isotropic elasticity tensor $\bar{C}_E^{\text{app}}(V)$ coincides with $\bar{\mu}_E^{\text{app}}(V)$, the ensemble average of the apparent shear moduli $\mu_E^{\text{app}}(V)$ defined by Equation (9) and computed for a domain V of given size (or equivalently containing $N = V$ grains in average). Accordingly, the estimation of $\bar{\mu}_E^{\text{app}}(V)$ only requires the determination of $\mu_E^{\text{app}}(V)$ for each realization. This is the computation strategy adopted in this work. Similarly, using SUBC conditions, it is sufficient to compute $\mu_\Sigma^{\text{app}}(V)$ for each realization according to Equation (10).

The apparent shear moduli and compliances $\mu^{\text{app}}(V)$ were computed using volume elements V of increasing size, ranging from $V = 25$ to $V = 5000$ grains, with $n(V)$ realizations for every volume. Number n is chosen such that the estimation of the mean $\bar{\mu}^{\text{app}}(V)$ is obtained with a precision better than 1%. This precision is estimated according to the simple sampling rule (13) involving the standard deviation $D_\mu(V)$. All simulation results are shown in Table 1.

Mean values and confidence intervals for the apparent shear modulus $[\bar{\mu}^{\text{app}}(V) - 2D_\mu(V), \bar{\mu}^{\text{app}}(V) + 2D_\mu(V)]$, are plotted in Figure 2, as a function of volume size V. The mean apparent shear moduli strongly depend on the domain size and on the boundary conditions. However, the values converge towards an asymptotic constant as the volume size increase, as expected (Sab, 1992). A striking feature of these results is the very fast convergence of the periodic solution and, in contrast, the very slow convergence associated with homogeneous boundary conditions. The periodic estimate is bounded by the KUBC and SUBC estimates:

$$\mu^{\text{Reuss}} \leq \bar{\mu}_\Sigma^{\text{app}} \leq \bar{\mu}_{\text{periodic}}^{\text{app}} \leq \bar{\mu}_E^{\text{app}} \leq \mu^{\text{Voigt}}, \tag{11}$$

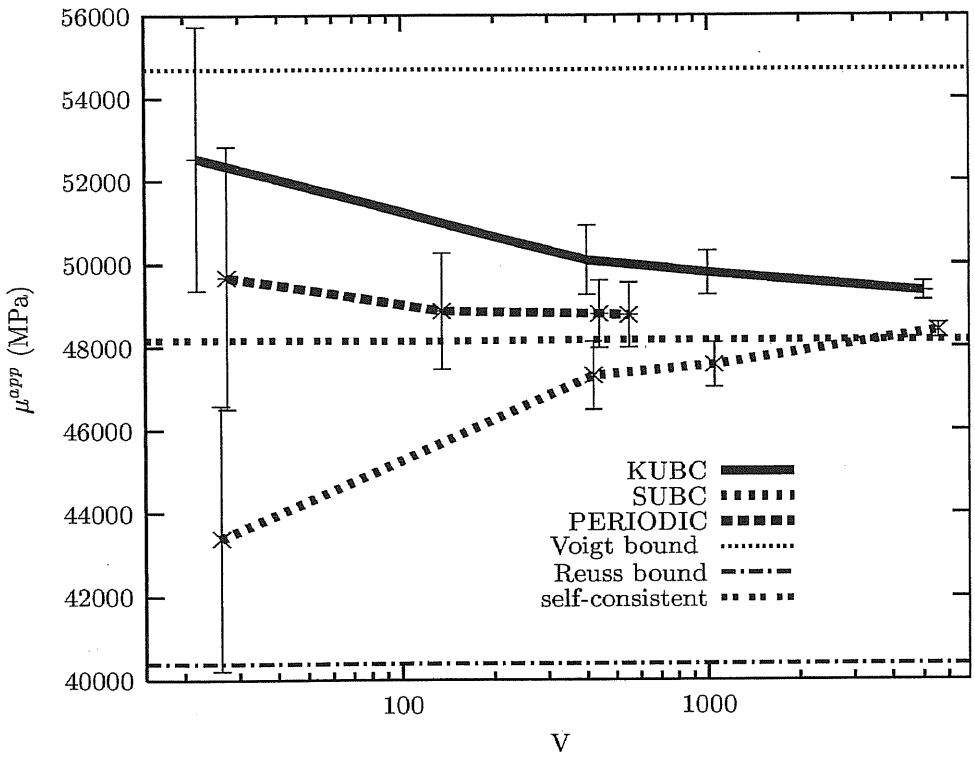

Fig. 2. Mean values and confidence intervals for the shear modulus μ^{app} as a function of domain size, for three different boundary conditions.

where μ^{Reuss} and μ^{Voigt} denote the first order lower and upper bounds for the effective shear modulus of the polycrystal (Zaoui, 1987). For decreasing values of V, the apparent moduli $\mu_E^{\text{Reuss}}(V)(\mu_\Sigma^{\text{Reuss}}(V))$ get closer to the upper (lower) limit $\mu^{\text{Voigt}}(\mu^{\text{Reuss}})$.

4 Determination of the Size of the RVE

The notion of RVE is necessarily related to the choice of a statistical precision in the estimation of the investigated effective property. First, we set a tolerance error α on the bias and find a corresponding volume V_0 such that:

$$|\bar{\mu}^{\text{app}}(V_0) - \mu^{\text{eff}}| \leq \alpha. \tag{12}$$

This condition sets a lower bound for the size of the RVE. Then, the relative precision of the estimation of the mean $\bar{\mu}^{\text{app}}(V)$ of apparent shear moduli for a given volume $V \geq V_0$ and a number of realizations n, can be defined according to the sampling theory by:

$$\varepsilon_{\text{rel}} = \frac{2D_\mu(V)}{\bar{\mu}^{\text{app}}(V)\sqrt{n}}. \tag{13}$$

In turn, the number of realizations required to correctly estimate $\bar{\mu}^{\text{app}}(V)$ is deduced from Equation (13) provided that the variance $D_\mu^2(V)$ is known.

According to homogenization conditions (8), (9) and (10), the apparent shear modulus is obtained by averaging an additive scalar over the volume V. As a result, it is shown by Matheron (1997) that, for asymptotically large volumes, the variance $D_\mu^2(V)$ of $\mu^{\text{app}}(V)$ is given by:

$$D_\mu^2(V) = D_\mu^2 \frac{A_3}{V}, \tag{14}$$

where A_3 is the integral range, a well-established quantity for additive geometrical properties such as volume fraction. D_μ^2 is the point variance of $C_{1212}(\underline{x})$, which depends on crystal orientation at x. For uniform orientation distribution, it can be expressed in terms of the single crystal cubic elasticity constants as follows:

$$D_\mu^2 = \langle (c : c)_{1212} \rangle - \langle c_{1212} \rangle^2 \quad \text{with} \quad \langle c_{1212} \rangle = \frac{1}{5}(C_{11} - C_{12} + 3C_{44}), \tag{15}$$

$$\langle (c : c)_{1212} \rangle = \frac{1}{35}(-6C_{44}C_{12} - 4C_{12}C_{11} + 2C_{12}^2 + 2C_{11}^2 + 6C_{11}C_{44} + 15C_{44}^2), \tag{16}$$

where $\langle \cdot \rangle$ refers to averaging over uniformly distributed orientations. For pure copper, one gets $D_\mu = 13588$ MPa. We choose to identify the integral range A_3 from the results obtained with periodicity conditions because they introduce the smallest bias in the estimated effective shear modulus. We find $A_3 = 1.43$, to be compared with the mean grain size set to 1, and the integral range for the volume fraction of a given orientation $A_3 = 1.17$ given by Kanit et al. (2003).

Equations (12), (13) and (14) can now be used quantitatively to determine a minimal size of RVE for a given precision ε_{rel} and a number of realizations n:

$$V = \frac{4}{n} D_\mu^2 \frac{A_3}{\varepsilon_{\text{rel}}^2 \mu^{\text{eff}\,2}}. \tag{17}$$

In the case of periodicity boundary conditions, the choice $(\varepsilon_{\text{rel}}, n) = (1\%, 10)$ gives a minimal volume corresponding to $V = 445$. For $n = 100$ successive computations, this volume reduces to 45.

5 Conclusions

A computational homogenization methodology was applied to the determination of RVE sizes for the isotropic linear elastic behaviour of copper polycrystals. For a given precision of 1% in the estimation of the effective property, and a number of affordable computations ranging from 10 to 100, RVE sizes remain of the order of 40 to 400 grains, provided that periodicity boundary conditions are applied to the polycrystalline aggregates. The convergence of apparent properties obtained using homogeneous boundary conditions towards the effective modulus is significantly slower than for periodicity conditions. The asymptotic shear modulus can be accurately estimated by a small number of huge computations or by a large number of small-scale computations, looking at the ensemble average of the apparent properties.

The integral range A_3 defined and identified in this work is a well-suited parameter to compare RVE sizes for different properties and morphologies. It characterizes the rate of decrease in the dispersion of apparent properties for increasing volume sizes, according to Equation (14). It depends on the investigated property (volume fraction, elasticity moduli, thermal conductivity, etc.). The value calculated in this work can be compared to the integral range found for a two-phase elastic material with a contrast in Young's moduli of 100 and 50% volume fraction of hard phase, namely $A_3 = 1.64$ (Kanit et al., 2003). The relatively high value found in the present work in spite of the relatively small contrast in properties between different orientations can be attributed to the multi-phase character of polycrystals, each crystal orientation being regarded as an individual phase. The volume must be large enough to contain enough individual orientations.

Acknowledgements

The authors are indebted to P. Featonby and J.-C. Leroy (SAGEM) for stimulating discussions during this work. The authors thank SAGEM and DGA for their financial and scientific support.

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Z-set package (2001) www.nwnumerics.com, www.mat.ensmp.fr.

A C.I.P. Catalogue record for this book is available from the Library of Congress.

ISBN-10 1-4020-5623-0 (HB)
ISBN-13 978-1-4020-5623-9 (HB)
ISBN-10 1-4020-5624-9 (e-book)
ISBN-13 978-1-4020-5624-6 (e-book)

Published by Springer,
P.O. Box 17, 3300 AA Dordrecht, The Netherlands.

www.springer.com

Printed on acid-free paper

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IUTAM Symposium on Mechanical Behavior and Micro-Mechanics of Nanostructured Materials

Proceedings of the IUTAM Symposium held in Beijing, China, June 27–30, 2005

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