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Microstructural numerical modeling of Al_2O_3/Ti composite

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Abstract

The present work focuses on the study of a numerical model of a ceramic/metal particle reinforced composite material that has the potential to be used in challenging engineering applications. The composite has been developed combining the specific properties of ceramic and metal in order to improve the overall mechanical characteristic compared to the characteristics of the individual materials only. In particular, the purpose of the composite is to improve the fracture toughness of the single ceramic in order to use it as protection against impact. Finite element modeling and analysis of a microstructure-based model have been used to analyze the mechanical behaviour of the particle reinforced composite in a virtual tensile test. The microstructure-based model has been created from scanning electron microscopy (S.E.M.) images identifying the areas and the edges of the two components present in the composite. The microstructure-based approach has been chosen for calculating the elastic properties starting from the material behaviour at the grain level in the ceramic and metal particles. The properties of the different individual particles have been used separately as the input to define the global mechanical properties of the composite.
The aim of this work is to create and validate the microstructure-based model by replicating the results available from experimental data for the elastic properties of the composite. Furthermore, the numerical results have been compared with analytical models for particle reinforced composites to have a wider knowledge of the capability of the model created.

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Keywords: Microstructured-based model; Numerical model; Elastic properties; Ceramic/metal composite

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1. Introduction

Materials for protection by impact have been strongly developed in the past decades both in material and constructive solutions. The direction of the improvement and the research in the design of protection is to develop solutions that are able to combine efficiency and weight reduction. The adoption of low-density materials (such as ceramic, composite, ballistic steel and titanium alloy) built in multi-layer systems has greatly contributed to the advances made. The combination of a hard-ceramic tile with a rear ductile plate are typically used and is able to respond to both the ballistic efficiency and the lightweight demand. However, the low fracture toughness of the ceramic plate can cause accidental breakage in harsh situations. The fracture toughness of ceramic can be improved by the incorporation of ductile metal particles into the brittle ceramic matrix, as in the Al_2O_3/Ti composite investigated in the present paper.

Currently the design and the study of material for personal protection is based mainly on experimental approaches that are very challenging, both in terms of cost and time; they are also affected by variability and uncertainty intrinsic to the phenomenon so that they usually require a wide sample of data to draw reliable conclusions. For this reason, it is worth to create an accurate and reliable method for the building of a numerical model that allows not only to predict the behaviour of the material and structures but also to minimize the experimental tests to be performed. Starting from the knowledge of experimentally obtained mechanical properties of the constituents and from their arrangement inside the composite in the research by Meir et al. (2015) and Hayun et al. (2016), the present work focuses on the numerical simulation of a static test aimed to acquire the basic mechanical properties of Al2O3/Ti. The scale in which the analysis is performed is on a micro-structural level of the composite.

Al_2O_3/Ti composite is fabricated from a mixture of Alumina powder (Ceralox, Tucson, AZ, high purity SPA-0.5, 0.5 μm) and titanium hydride TiH_2 powder (Alfa Aesar, Ward Hill, MA, 99% metal basis, 325 mesh). The powders are blended in a planetary ball mill inside a polyethylene container for three days with ethanol and alumina milling balls. Titanium hydride is preferred to pure titanium powder because the latter leads to the formation of inter-metallic compounds and oxides on the metal/ceramic interface that weaken the grain boundaries and lead to decreased mechanical properties. The powder mixture is processed with spark plasma sintering (SPS) to obtain the composite material. The S.E.M. analysis in Meir et al. (2015) showed that the titanium particles are crushed and homogeneously dispersed in the alumina powder.

The advance of computation capacities in the last decades has aided the finite element method, in particular the development of numerical models representing micro-structural schemes of different kinds of composite materials. Wolodko et al. (2000) investigated the material behaviour at the micro-structural level to gain a better understanding of the influence of the micro-mechanical mechanisms such as friction between the phases and of the fiber/particle shape and distribution on the composite properties. Balasivanandha Prabu et al. (2008) focused their attention on the numerical definition of the interface between the fiber/particles and the matrix to recreate the detachment between these two components.

In section 2 a microstructure-based finite element model with the aim to calculate the elastic properties of the composite starting from the mechanical properties of the constituents is presented. Several methods to obtain reliable data for the comparison with experimental tests are herein investigated

In section 3 an analytical approach for the assessment of the elastic properties of a two-phase material is introduced and the analytical, numerical and experimental values of the elastic properties of the composite are compared. The conclusion and potential future developments are reported in section 4.

2. Microstructured-based numerical model

In this section, the building of a microstructure-based finite element model consisting of two distinct components: metal and ceramic particles is introduced and presented. A method for extrapolating and creating the geometrical model starting from SEM pictures on the composite is given. The microstructure-based analysis allows to simulate the behaviour of the material at the scale of the phases, the alloy components or the constituents. The main advantage of this approach is to evaluate the influence of the microscopic scale phenomena, e.g. the distribution and the shape of the reinforcing particles, the friction between different the phases, etc. on the response of the composite material at a macroscopic scale. However, the use of this scale for further applications is not straightforward, therefore the gathering of the mechanical properties of the whole composite is a first step for the exploitation of this material in the simulation at a higher scale.

As anticipated, this work includes the simulation of a tensile test on a metal/ ceramic particle-reinforced composite made of alumina and titanium, Al_2O_3/Ti, at various levels of ceramic to metal ratio in order to get elastic properties; the experimental data for comparison were obtained from Meir et al. (2015) and Hayun et al. (2016).

The description of the material behaviour as a composite is derived from the response of the two constituents: alumina and titanium. The information required was taken from Hayun et al. (2016) for Alumina (Ceralox, Tucson, AZ, high purity SPA-0.5, 0.5 µm) and titanium hydride TiH_2 (Alfa Aesar, Ward Hill, MA, 99% metal basis, 325 mesh). The models chosen to represent the elasto-plastic and the damage behaviour are Johnson-Cook for titanium and Johnson-Holmquist for alumina. At this level only the elastic mechanical properties are investigated, however the use of a more complete description of the mechanical behaviour of the material is functional to further development of the method. Both alumina and titanium require a particular production process and consequently the literature lacks some specific constants including the damage and the dynamic constant; these values were therefore taken from the most similar material available in the literature. The values for high purity titanium (99.999%), listed in Table 1, are from Hayun et al. (2016), Revil-Baudard B. et al. (2011), Varmint (2014). The values for Alumina (Alumina high purity SPA-0:5, 99.995%) listed in Table 2 are from Hayun et al. (2016), Johnson G. R et al. (1994).

Table 1. Parameters for the Johnson-Cook model for titanium

Density	ρ	4.52 kg/dm3
Young's modulus	E	122000 MPa
Poisson's ratio	ν	0.32
Static yield stress	A	236 MPa
Hardening modulus	B	245 MPa
Hardening coefficient	n	0.539
Strain rate coefficient	C	0.0125
Effective plastic strain at failure	PSFAIL	1.2483

Table 2. Parameter for Johnson-Holmquist model for alumina 99.995%

Density	ρ	3.95 kg/dm3
Shear modulus	G	178000 MPa
Young's modulus	E	420000 MPa
Poisson's ratio	ν	0.18
Fractured normalized strength parameter	B	0.31
Strength parameter (for strain rate dependence)	C	0
Fractured strength parameter (pressure exponent)	M	0.6
Intact strength parameter (pressure exponent)	N	0.6
Quasi-static threshold strain rate	EPSI	1
Maximum tensile pressure strength	T	200 MPa
Maximum normalized fractured strength	SFMAX	0.2
Hugoniot elastic limit	HEL	8800 MPa
Pressure component at Hugoniot elastic limit	PHEL	1460 MPa
Bulk factor	β	1

Parameter for plastic strain to failure	D1	0.005
Parameter for plastic strain to failure (exponent)	D2	1
First pressure coefficient (bulk modulus)	K1	218750 MPa
Second pressure coefficient	K2	0
Third pressure coefficient	K3	0

A bi-dimensional model can be developed, as done in Balasivanandha Prabu et al. (2008), from the images of the scanning electron microscopy (S.E.M.) with the resolution and size that allows the recognition of two or more phases of the composite and to have a reference surface which is wide enough. The sequence of the creation of the numerical model is reported in Figure 1. Image segmentation is the process of partitioning a digital image into multiple segments or sets of pixels: this process is done by Fiji, an open-source software of image processing. It is used in this context with the purpose to identify and localize the objects and boundaries in the image assigning a label to every pixel, therefore pixels with the same label share certain characteristics and it is then possible to graphically separate the two phases. The areal ratio (ceramic to metal particles) can be also calculated. Vectorization, by means of Inkscape TM open source software and the creation of the numerical model is subsequently done by FRECAD. The complete sequence is depicted in Figure 1.

The mesh of the matrix and the reinforcing particles was created using the finite element software Abaqus/CAE, however LS-DYNA was selected as a solver. The 2D model was constructed with a free mesh and quad four node elements and the resulting size of the model is 0.0234 mm x 0.0159 mm. The dimension of the element (6.3E-5 mm) was chosen as the best trade-off

- between the most accurate description of the geometry of the interface between the matrix and the reinforcing particles.
- to reduce the computational time
- to keep the nodes of the elements of the matrix as close as possible to the reinforcing particles on their interface.
- convergence analyses were also performed.

The aim of this work is the simulation of a virtual tensile test on the composite material in order to obtain the elastic properties of the assembly; the schematization of the test is shown in Figure 2. The constraint was chosen to replicate the plane strain condition of the slice of the material in the central part of the virtual specimens (at the grain level). All the simulations were performed under the plane strain hypothesis with a prevented deformation in the z direction; the connection between the stress and the strain in the x direction was subsequently expressed by an apparent Young's modulus E'. The Young's modulus was then calculated from the linear elastic relationship for the isotropic material under the plane strain hypothesis. Finally, the finite element model is shown in Figure 3. It is worth mentioning that precisely meshing the interface avoiding inter-penetration or voids between the elements is not straightforward. The elastic properties of alumina and titanium are assigned to blue and red particles, respectively and a quasi-static analysis was run. The metal and ceramic particles are constantly in contact and their stiffness influences the shape and the stress at the interface. In this work, due to the low stress level, the contacts were hypothesized as perfect bonding.

However, the aim is to replicate the results of the experimental tests performed in Hayun et al. (2016) through the present microstructure-based model. In Hayun et al. (2016) the elastic properties were evaluated experimentally with an ultrasonic pulse-echo technique, following the reference standard ASTM D-2845. The reference standard ASTM D-2845 states that the values of the elastic constants obtained by an ultrasonic pulse-echo test often vary from values determined by static laboratory methods (tensile test, triple bending, etc.), however an ultrasonic test offers a good approximation and a useful preliminary prediction of the static properties. Thus, in the numerical model herein presented the elastic properties were obtained by mimic the ultrasonic pulse-echo techniques, inside the virtual environment of the model, and by comparing the results obtained with the experimental data. In Weglewski W. et al. the elastic constants of a metal matrix and ceramic reinforcing particles composite manufactured by Spark Plasma Sintering were assessed in four different ways including an ultrasonic pulse-echo technique and a tensile test on a finite element model, built up from a micro-tomography of the composite material. The Young's modulus value from the ultrasonic test results was 5% higher compared with the tensile test value; In Miyazaki M. (2002) the authors compared the Young's modulus value in tensile and ultrasonic tests on brittle material (dentin) showing that on average the two values, for the same specimen, differed by 22%. Also Balasivanandha Prabu et al. (2008) showed differences between static tensile and ultrasonic tests around 20% due to a variation of the micro-structures in the test specimen and the presence of micro-voids that influenced the tests.

The results are reported in Table 3. The finite element simulation of the elastic properties of the composite confirmed a lower stiffness which proves previous works, papers and the standard ASTM D-2845

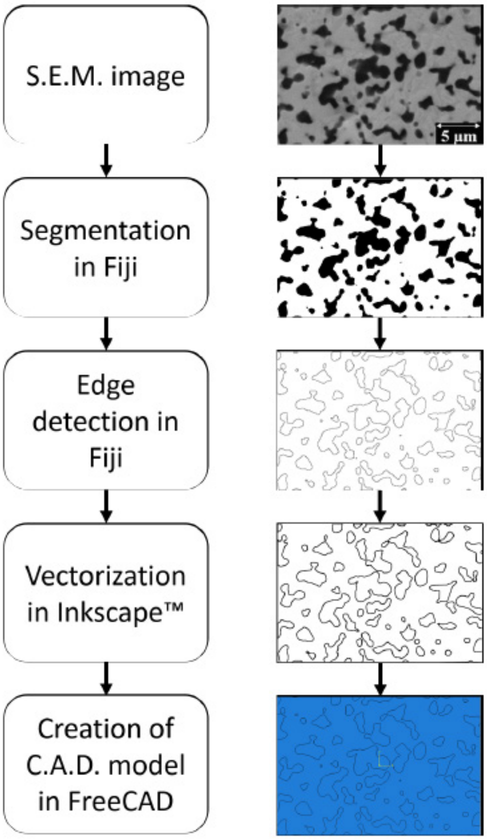

Fig. 1. Sequence of the creation of the numerical models starting from SEM image

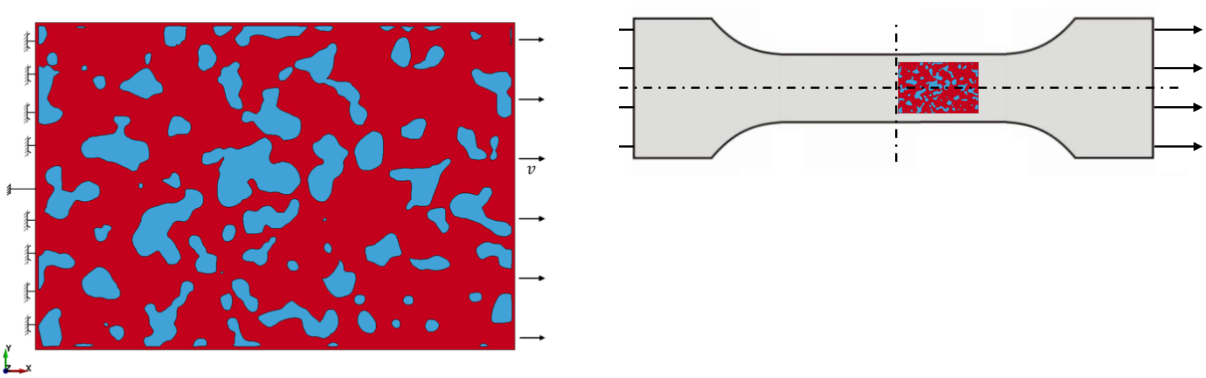

Fig. 2. Boundary condition of the model

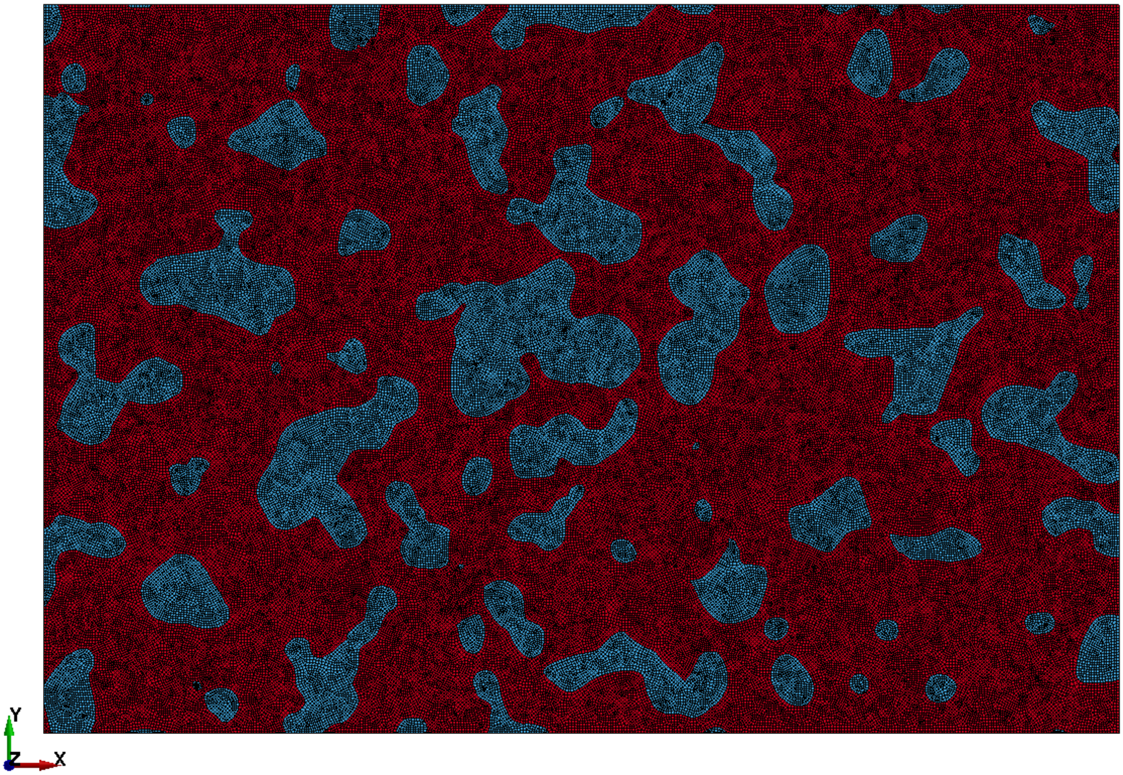

Fig. 3. The finite element model of the representative area

Table 3. Results for the composite model

Al_2O_3/Ti composite with 20% weight fraction of alumina

	Experimental	F.E.M.	Error %
E' [MPa]	− − −	175960	− − −
ν	0.28	0.27	-3%
E [MPa]	187000	162146	-13%

The ultrasonic pulse-echo technique test can be simulated numerically. The longitudinal modulus (also named P-Wave or constrained modulus) is the ratio of the axial stress to the axial strain in a uniaxial strain state. It is equivalent to a Young's modulus without transverse strain. It can be expressed as:

$$M = \frac{\sigma_x}{\varepsilon_x} \tag{1}$$

when $\varepsilon_y = \varepsilon_z = 0$.

This quantity can also be extrapolated from the numerical simulation through the longitudinal wave velocity v_l:

$$M = \rho v_l \tag{2}$$

From the knowledge of the longitudinal modulus, here calculated, and the Poisson's ratio, the elastic Young's modulus can be estimated as follow:

$$E = M(1+\upsilon)(1-2\upsilon)/(1-\upsilon) \tag{3}$$

This calculation provides an assessment of the Young's elastic modulus which is 193383 MPa; this value is closer (3% error) to the experimental value reported in Hayun et al. (2016).

3. Analytical model and comparison

Many theoretical models have been developed to describe and predict the elastic properties of two-constituent's materials. All of the models require the properties of the single phases as input and start with the assumption that the two-constituents' materials are homogeneous on a scale much larger than the size of the inclusions, and that the displacement and traction at the interface between the two phases are continuous.

The experimental data vary within a range and the capability of the model predictions to provide upper and lower bounds to cover the experimental data seem more plausible. Therefore, the following three models were chosen: Voigt–Reuss (Voigt W. (1889), Reuss A. (1929)), Hashin–Shtrikman (H–S model, Zimmerman R.W (1992)) and Ravichandran models (Ravichandran K. S. (1993)).

In this sectiona comparison between experimental, analytical and numerical results for the elastic constants is presented. The experimental values were taken from Meir et al. (2015) and Hayun et al. (2016) and different densities were considered. Accordingly, the numerical and analytical models were built.

As far as numerical models are concerned, their building was started by the SEM images at different densities: 20% (already calculated), 40%, 60%, 80%.

Assuming a constant thickness for both reinforcing particles and matrix is possible the conversion from weight to areal ratio and compare these figures with the data obtained during the building of the FE model (starting from SEM images), Table 4. It's worth to mention that the nominal ceramic to metal ratio (in weight) is not always respected in the SEM images and a lower fraction of alumina particles is present in the composite. The reason for this discrepancy between the value from Hayun et al. (2016) and the calculated one could be multiple. The nominal value is referred to the initial ratio between the powders and during the process of sintering it is possible that a small amount of material is transformed into an unwanted phase like TiH_2 or Ti_3Al. Another explanation could be that the S.E.M. images does not replicate the representative area of the composite.

Table 4. Al_2O_3/Ti composite weight fraction of alumina

Theoretical Alumina weight fraction	Theoretical Alumina areal fraction.	Measured Alumina areal fraction
0.2 (20%)	0.222	0.20
0.4 (40%)	0.433	0.333
0.6 (60%)	0.632	0.47
0.8 (80%)	0.821	0.79

Finally, elastic properties obtained from the numerical models are reported in Figure 4. The Young's modulus calculated numerically is lower than the experimental one; this difference has a twofold cause:

- the experimental values, taken from Hayun et al. (2016) were extrapolated by an ultrasonic pulse-echo technique that usually provides more rigid values compared with than the numerical tensile test values. Analytical and numerical models were, on the contrary, calculated on the mechanical behaviour of the structure;
- as previously stated, the actual ceramic to metal ratio of the model is in some cases sensibly lower than the nominal one; in fact, 40% and 60% show greater discrepancy whereas the error for the 80% is similar to the case of 20%.

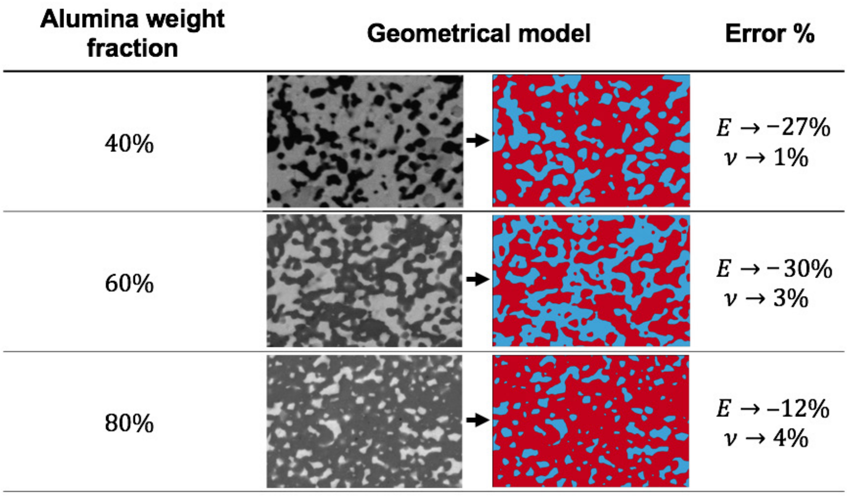

Fig. 4. Results for the composite model for different percentage of weight fraction of alumina

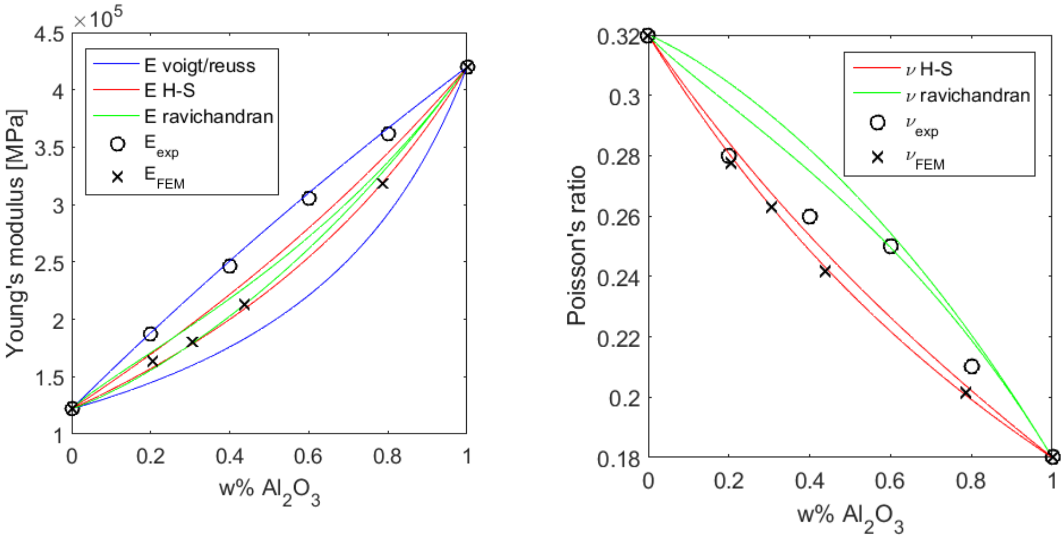

Fig. 5. Comparison between the experimental, analytical and numerical results for the elastic constants as a function of the fraction of Alumina

Figure 5 shows the comparison between the experimental, analytical and numerical results for the elastic Young's modulus. The numerical values seem to follow the lower boundary of the H-S and the Ravichandran models.

4. Conclusion

The results presented show a good agreement with the experimental data especially when the results form numerical modelling approaches were obtained using the same method used in the experimental tests. The elastic properties were chosen, as a target to be replicated, due to experimental data available for comparison. Good replication was achieved for the Poisson's ratio with a percentage error around 3%. For the elastic Young's modulus, the percentage error between the numerical results and experimental data was higher but this discrepancy can be explained by the difference in the calculation of the elastic properties between the experimental (ultrasonic pulse-echo technique) and the numerical (virtual tensile test) procedure and by a mismatch between actual ceramic to metal ratio in SEM images. For the first issue a relevant improvement in the prediction of the experimental data was achieved when data exploiting the stress wave method was investigated also in the numerical methods.
It is worth mentioning that, even if the elastic properties are only a small amount of data for the characterization of the mechanical behaviour of the material, the present method could be used also for the replication of more complex data starting from constituents. This could allow a prediction of the mechanical properties as a function of a fraction of the constituents.

The next steps in this work could be the assessment of the goodness of the calibration, here performed, by means of a numerical replication of more complex tests, like dynamic tests. Moreover, also the interaction between the two constituents can be further investigated. The final aim could be the creation of a reliable and efficient method to simulate impact tests with the coexistence of both micro-structured and macro-structured models and therefore performing advanced numerical simulations, like the optimization of the material up to impact event.

References

Balasivanandha Prabu S. and Karunamoorthy L.. "Microstructure-based finite element analysis of failure prediction in particle-reinforced metal-matrix composite". In: Journal of Materials Processing Technology vol 207 issue .1-3 (2008), pp. 53–62..

Johnson G. R. and Holmquist T. J. "An improved computational constitutive model for brittle materials". In: AIP Conference Proceedings 309.1 (1994), pp. 981.

Hayun S. et al. "Phase Constitution and Dynamic Properties of Spark Plasma-Sintered Alumina-Titanium Composites". In: Journal of the American Ceramic Society Volume 99, Issue 2 (2016), Pages 573–580

Meir S. et al. "Mechanical properties of Al_2O_3nTi composites fabricated by spark plasma sintering". Ceramic International 41 (2015) 4637 - 4643

Miyazaki M. "Use of an ultrasonic device for the determination of elastic modulus of dentin". In: J Oral Sci 44.1 (2002), pp. 19–26.

Ravichandran K. S.. "Elastic Properties of Two-Phase Composites".In: Journal of the American Ceramic Society, Volume 77, Issue 5 (1994), pp. 1178–1184

Reuss A. "Berechnung der Fließgrenze von Mischkristallen auf Grund der Plastizitätsbedingung für Einkristalle ." en. In: ZAMM - Zeitschrift für Angewandte Mathematik und Mechanik 9.1 (Jan. 1929), pp. 49–58

Revil-Baudard B. et al.. "Plastic deformation of high-purity -titanium: Model development and validation using the Taylor cylinder impact test". In: Mechanics of Materials 80. (2011), pp. 264–275.

Standard D2845-05 ASTM. "Standard Test Method for Laboratory Determination of Pulse Velocities and Ultrasonic Elastic Constants of Rock". (2005), pp. 5–11.

Varmint. Varmint Al's. 2014. url: http://www.varmintal.com/aengr. htm%7B%5C#%7DMats-for-LS-DYNA

Voigt W. "Ueber die Beziehung zwischen den beiden Elasticitätsconstanten isotroper Körper". In: 274.12 (1889), pp. 573–587. issn: 15213889.

Weglewski W. et al.. "Comparative assessment of Young's modulus measurements of metal-ceramic composites using mechanical and non-destructive test and micro-CT based computational modeling". In: Computational Materials Science, Vol 77 (2013), pp. 19–30

Wolodko J. D., Xia Z., and Ellyin F.. "Analysis of Al/Al2O3 metal matrix composites under biaxial cyclic loading using a digital image based finite element method". In: Materials Science and Technology 16.7-8 (2000), pp. 837–842.

Zimmerman R.W.. "Hashin–Shtrikman bounds on the Poisson ratio of a composite material". In: Mech. Res. Commun. 19 (1992), pp. 563–569