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The Effective Elastic Modulus of Laser-Engineered Composite Boride Coating**

By T. Laha, A. Agarwal,* and N. B. Dahotre

Small and hard second phase particles distributed randomly in a ductile matrix are a common source of material strengthening because of the effect of higher strength and the restriction of grain growth of matrix. The prediction and estimation of the change in overall mechanical properties (e.g. elastic modulus, hardness etc.) of random heterogeneous materials are of great interest to researchers and engineers in many science and engineering disciplines. Definite values of overall effective properties are being estimated for the given geometry of the constituents which are based on explicit formulae or the values can be defined by the use of the upper and lower bounds.

Several efficient approaches have been proposed in order to predict the effective elastic modulus. Eshelby's solution has been proved to be an efficient method to compute this for composites with ellipsoidal heterogeneity embedded in a linearly elastic infinite matrix.^[1-3] The elastic moduli tensors are uniform both within the ellipsoid and uniform within the matrix in this case.^[1-4] Another method that has been used extensively to estimate this property is the Mori-Tanaka mean-field theory where the inclusions with ellipsoidal shape have

been assumed to be either aligned or randomly dispersed in the matrix and both the inclusions and matrix follow linear elasticity.^[1-2,5-8] This model has proven to be quite accurate in predicting the effective properties of various materials with either random orientation or total alignment of the reinforcing phases. The Hashin-Shtrikman variational principle is widely used for the prediction of the effective properties of linearly elastic composite materials.^[1,2] This variational principle yields upper and lower bounds for the effective properties instead of one modulus value, when the volume fraction of heterogeneities is given. Since the effective properties are the overall responses of material samples subjected to uniform boundary conditions, the variational principle can be generalized to solve a general boundary value problem for a heterogeneous body. When the body is linearly elastic, the generalized variational principle determines two bodies, which overestimate and underestimate the expectation of the total strain energy. The analysis of these bodies provides upper and lower bounds for the expectation.^[1,2, 9-12]

In the present work, the overall effective elastic modulus of the laser-engineered composite TiB₂ coating has been computed using Eshelby's approach, Mori-Tanaka method and the Hashin-Shtrikman bound method. The effective elastic modulus of TiB₂ composite coating has been estimated in our previous work^[13] using the rule of mixture (ROM), where the elastic modulus of second phase TiB₂ particle and the Fe-rich matrix were measured by nanoindentation technique. A comparison of effective elastic modulus of the coating estimated by the various micromechanics models has been made in this work.

Synthesis and Characteristics of TiB₂ Coating: The composite TiB₂ coating was synthesized by depositing a low density and ultrahard TiB₂ ceramic (which possesses excellent wear and oxidation resistance) on AISI 1010 steel substrate using Laser Surface Engineering (LSE) process.^[14] The coating, metallurgically bonded to the steel substrate is composite in nature, with TiB₂ particles of various sizes and shapes embedded in Fe-rich matrix.^[13,14] The detailed procedure of coating formation is reported elsewhere.^[14] Three different TiB₂ coatings (B1, B2, B3) with different volume fraction (0.52, 0.66 and 0.69 respectively, Tab. 1) were obtained by varying the laser traverse speed. The interaction time of the laser beam decreases with the increasing

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Table 1. Volume fraction, and experimental and literature values of elastic modulus of TiB₂ and Fe-rich matrix.

Sample	Volume fraction		Elastic modulus (GPa)			
	TiB ₂	Matrix	TiB ₂		Matrix	
			Expt.	Lit.	Expt.	Lit.
B1	0.52	0.48	558.6	551.5	326.4	236.3 (1010 steel)
B2	0.66	0.34	556.9		306.4	
B3	0.69	0.31	560.3		292.4	

Table 2. Primary features and assumptions of the various micromechanics models in estimating the effective elastic modulus.

Assumption	Eshelby's Approach	Mori-Tanaka Method	Hashin-Shtrikman Bound Method
Concentration of particulates	Dilute	Non-dilute	Independent of concentration
Matrix	Linearly elastic	Linearly elastic	Linearly elastic
Shape of particulates	Ellipsoidal (assumed spherical in this paper)	Ellipsoidal (assumed spherical in this paper)	Independent of shape

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laser traverse speed, resulting in different volume fraction of TiB_2 in the coating. Detailed microstructural characterization along with quantitative microscopy of B1, B2 and B3 has been performed and presented elsewhere.^[14] The SEM micrograph of B3 sample shows crack free, metallurgically bonded coating in Figure 1. X-Ray Diffraction analysis of the TiB_2 -coated steel surface indicated TiB_2 as the major phase with a few small peaks of metastable phases of type Fe_aB_b and Ti_mB_n that formed due to high cooling rate involved during laser processing.^[13-16] TEM micrograph and corresponding EDS analysis and SAD pattern corroborated the Fe-rich matrix containing fine dendrites and ultrafine dissolved boride particles.^[3,10] The estimation of effective elastic modulus values by nanoindentation technique justified that this dissolution of TiB_2 and metastable phases increases the elastic modulus of the Fe-rich matrix to 1.5 times higher than the theoretical value of AISI 1010 steel. The values of effective elastic modulus obtained from nanoindentation technique and using ROM are listed in Table 1.^[13]

Theoretical Models to Estimate Elastic Modulus: A comparison of different theoretical models used to estimate the effective elastic modulus in the present study has been done in Table 2. All the methods assume the matrix as well as the second phase are linearly elastic. Eshelby has considered an ellipsoidal inhomogeneous inclusion embedded in an infinite matrix.^[1-4]

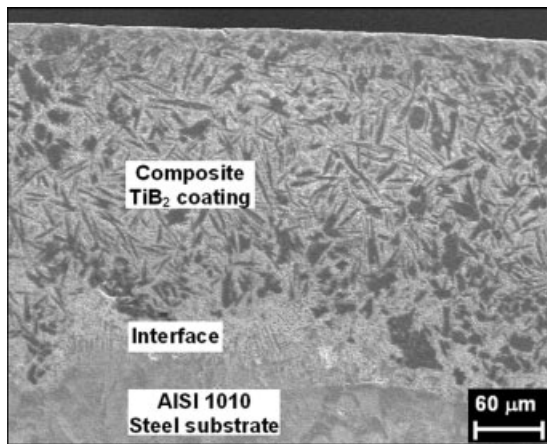


Fig. 1. SEM micrograph showing cross-sectional view of laser surface engineered composite TiB_2 coating on AISI 1010 steel substrate

In the present study the TiB_2 particles can also be treated as inhomogeneities embedded in Fe-rich matrix because of the difference in elastic moduli of TiB_2 and the Fe-rich matrix. The equivalent inclusion method is assumed in this approach to simulate the stress disturbance due to the presence of TiB_2 particles in Fe-rich matrix whereas the TiB_2 particles as well as the Fe-rich matrix are considered as linearly elastic materials. The ellipsoidal shape covers a wide variety of shapes i.e. cylinders, spheres, elliptic, penny-shaped or ribbons. In the present study the shape of the TiB_2 particles is assumed to be spherical shape for the sake of simplicity in computation. In fact, the shape of the TiB_2 particles changed from polygonal to acicular / needle shape with the increase in laser traverse speed.

The effective elastic modulus of the boride composite coating is also estimated by using the Mori-Tanaka mean-field theory. It is assumed that both the TiB_2 particles and the Fe-rich matrix behave linearly elastic during applying load in nanoindentation technique.^[13] Benveniste et al. found that if the "typical inclusions" are embedded as second phase particulates in the matrix then the Mori-Tanaka stiffness tensor is symmetric.^[6] Thus, Mori-Tanaka method can be applied to compute the effective elastic modulus of the composite coating where TiB_2 particle are dispersed in Fe-rich matrix. As the volume fraction of second phase TiB_2 particles is reasonably higher (> 50 %) in all the three different coatings, the system was considered as non-dilute concentration of reinforcement which satisfy the condition for achieving consistent effective elasticity values.^[17]

Hashin-Shtrikman bound method is independent of shape of phase region or crystallites. Therefore, the shape of TiB_2 particles is not a subject of concern in this case. Depending upon the volume fraction of TiB_2 particle, a range of effective elastic modulus values of the composite coating is obtained by this method.

Results and Discussion: The effective elastic modulus values of the composite TiB_2 coating have been computed applying ROM by using the elastic moduli of TiB_2 and Fe (matrix) obtained from literature and nanoindentation technique (Tab. 3) and have been plotted in Figure 2. It is evident from Figure 2 that the effective elasticity values computed by nanoindentation technique possess higher value than the theoretical values. These higher vales are attributed to the dissolved TiB_2 particles and traces of metastable phase(s) in the Fe-rich matrix. The

Table 3. Comparison of different methods in respect with effective elastic modulus (GPa).

Sample	Rule of Mixture (Nano indentation) [13]	Rule of Mixture (Literature value) [13]	Eshelby's Approach	Hashin-Strikmann Bound		Mori-Tanaka Method
				Lower limit	Upper limit	
B1	447.14	400.20	402.46	423.80	432.51	415.28
B2	471.73	444.33	424.42	459.97	468.30	451.56
B3	477.25	453.79	428.92	468.05	476.07	459.86

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values of effective elasticity estimated by different micromechanics models (i.e. Eshelby's approach, Mori-Tanaka method and Hashin-Shtrikman bound method) are reported in Table 3 and plotted in Figure 2.

It can be observed from Figure 2 that the effective elastic modulus values obtained from Eshelby's approach possess lower values than those obtained by applying ROM with the values from nanoindentation technique and literature. This discrepancy is attributed to the higher volume fraction of second phase TiB₂ particles in the matrix (non-dilute composite structure), whereas for dilute system Eshelby's method evaluates consistent values of effective elastic modulus (Fig. 2).^[3,17] The graph shows that this discrepancy increases with the increase in volume fraction of TiB₂ particles. It was noticed earlier^[14] that B2 and B3 samples result in uniform distribution of TiB₂ particles in the melt zone whereas sample B1 shows non-uniform distribution. The shape of the TiB₂ particles also changed from polygonal to acicular/needle shape. This uniformity and change in shape was experienced more in B3 samples i.e. with the increase in laser traverse speed.^[14] The discrepancy in elastic modulus values obtained by using Eshelby's Approach and nanoindentation technique is also attributed to this uniformity and change in shape of TiB₂ particles.

The effective elastic modulus values obtained from Mori-Tanaka method show consistent result with the values obtained by nanoindentation technique. It can be noticed from Figure 2 that the values obtained by this method shows

disparity with the values obtained by applying nanoindentation technique at lower volume fraction of TiB₂ particles. However, the disparity minimizes with increase in volume fraction of TiB₂ particles. This behavior justifies the compatibility of the results obtained by Mori-Tanaka method for non-dilute composite materials.^[17] It is clear from Figure 2 that the Mori-Tanaka method is more reliable than Eshelby's approach in estimating effective elastic modulus.

Effective elastic modulus values obtained from Hashin-Shtrikman bound method resembles well with the values obtained by nanoindentation technique. The TiB₂ particles were assumed as spherical during calculating effective elastic modulus by both Eshelby's approach and Mori-Tanaka method. However, Hashin-Shtrikman bound method is independent of the shape of the second phase TiB₂ particles. Therefore, the change in shape of TiB₂ particles to acicular shape with the increase in laser traverse speed did not affect the values of effective elastic modulus of the composite coating. In addition, this micromechanics model is valid for higher concentration of the second phase. Therefore, effective elastic modulus values estimated using this model provide a good match with the values obtained by nanoindentation technique for different TiB₂ volume fraction.

Conclusions: Micromechanics models (e.g. Eshelby's Approach, Mori-Tanaka Method and Hashin-Shtrikman Bound Method) provide efficient and reliable alternatives to estimate effective elastic modulus of laser surface engineered TiB₂ coating on AISI 1010 steel substrate.

Effective elastic modulus values estimated by Eshelby's approach are lower compared to other methods, which is attributed to the higher volume fraction of TiB₂ particles and the presence of acicular shaped TiB₂ particles with increase in laser traverse speed.

Mori-Tanaka method shows consistency with the nanoindentation technique, which increases with increase in volume fraction of TiB₂ particles.

Hashin-Shtrikman Bound method yields most consistent effective elastic modulus values of the TiB₂-coated AISI 1010 steel substrate which is attributed to the independence of this method to geometry and volume fraction of second phase TiB₂ particles.

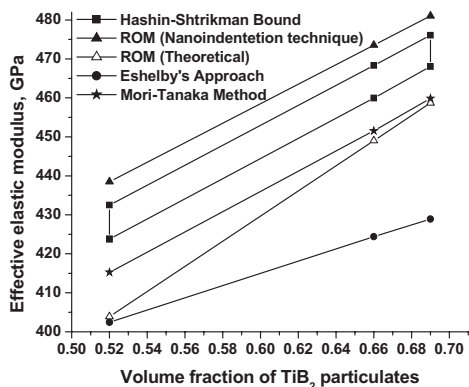


Fig. 2. Comparison of effective elastic modulus for different volume fraction of TiB₂ particles estimated by different methods.

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Surface Modification of Pure Ti by Laser Alloying with B and Ni Mixed Powders**

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Titanium and its alloys are extensively used in aeronautical, marine and chemical industries due to their intrinsic properties such as high strength, good oxidation and corrosion resistance. Nevertheless, the applications of titanium alloys under severe wear conditions are currently restricted due to their low hardness and poor tribological properties. In addition, titanium alloys present limited oxidation and corrosion resistance at high temperature because of their strong affinity towards oxygen at elevated temperature in air.

Surface modification can enhance the properties of titanium alloys. But conventional chemical heat treatments such as nitriding, carburizing and boronizing have some disadvantages such as long processing time, thin treated layer and easy deformation of the workpiece being treated. Spray coatings also have some demerits such as low coating density and limited bond strength between the coating and the substrate. Laser beams, owing to their good coherence and directionality, are widely used in surface modification of many kinds of metals. So, the disadvantages of pure titanium and its alloys can be overcome by laser surface modification treatment of the special surfaces of the workpieces where they suffer in operation. Laser treatment has several advantages over commonly used heat treatment methods, including precise control over the width and depth of processing, ability to selectively process specific areas of a component, and ability to process complex parts.

Laser nitriding of titanium alloys is a common way for improving their wear and corrosion resistance. The wear resistance of laser nitrided Ti-6Al-4V alloy is enhanced noticeably under both two-body abrasive and dry sliding

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