Micromechanical Modelling of Thermoelastic Behavior of AA7020/TiC Metal Matrix Composites

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Abstract: ***The present work was intended to estimate thermoelastic behavior of AA7020/titanium carbide nanoparticle metal matrix composites. TiC is used as a heat shield coating for atmospheric reentry of spacecrafts. The thermal loading was varied from subzero temperature to recrystallization temperature. The RVE models were used to analyze thermo-elastic behavior. The stiffness of AA7020/titanium carbide nanoparticle metal matrix composites increased with the increase of temperature and loading of TiC nanoparticles. The stiffness was raised steeply above 100°C which is very interesting phenomena to be scientifically explored for low volume fractioned (20%) TiC composites. A higher modulus characteristically indicates that the material is harder to deform.***

Keywords: AA7020 alloy, titanium carbide, RVE model, thermoelastic, finite element analysis

1. Introduction

To deal with the apparent confines of monotonic alloys, for instance, low stiffness and low strength, and to expand their applications in variety of sectors, nanoparticulate fillers, such as SiC [1-7], Al_2O_3 [8-12], Si_3N_4 [13], carbon [14], $Al(OH)_3$ [15] are often added to process metal matrix composites, which usually unite the compensation of their constituent phases. Titanium carbide (TiC) has elastic modulus of approximately 400 GPa, shear modulus of 188 GPa and CTE (coefficient of thermal expansion) of 7.4 μm/m-°C. TiC is employed as an abrasion-resistant surface coating on metal parts, such as tool bits and parts of timepiece mechanisms. TiC is also used as a heat shield coating for atmospheric reentry of spacecrafts. AA7020 alloy has elastic modulus of 71.7 GPa, shear modulus of 26 GPa and CTE of 7.4 μm/m-°C. AA 7020 alloy is used for motorbike or bicycle frames and armored vehicles.

The present work was intended to build up nanoparticulate TiC/AA7020 alloy matrix composites. Because the constituents have very different modulus and CTE, the internal stress inhomogenity can swiftly raise even under a low level of external applied loads or changes in temperature [16]. For that reason, it was indispensable to be aware of the thermo-elastic behavior of TiC/AA7020 alloy nano metal matrix composites. Finite element method (FEM) was exercised to measure the local response of the material using unit cell reinforced by a single particle subjected to periodic and symmetric boundary conditions [18].

2. Material and Methods

The matrix material was AA7020 alloy. The reinforcement nanoparticulate was TiC of average size 100nm. The mechanical properties of materials used in the current work are given in table 1. The volume fractions of TiC nanoparticles were 20% and 30%.

Table 1: Mechanical properties of AA7020 matrix and TiC nanoparticles

Property	AA7020	TiC
Density, g/cc	2.83	4.93
Elastic modulus, GPa	71.7	497
Ultimate tensile strength, MPa	524	119
Poisson's ratio	0.33	0.19
CTE, μm/m-°C	21.7	7.4
Thermal Conductivity, W/m-K	157.0	330
Specific heat, J/kg-K	860	565

In this investigation, a square (representative volume element) RVE (figure 1) was outfitted to interpret the thermo-elastic (compressive) behavior AA7020/ TiC nanocomposites. The PLANE183 element was used in the matrix and the interphase regions in the RVE models. The interphase between nanoparticle and matrix was discretized with CONTACT172 element [19]. The maximum contact friction stress of $\sigma_y/\sqrt{3}$ (where, σ_y is the yield stress of the material being deformed) was enforced at the contact surface. Both uniform thermal and hydrostatic pressure loads were applied simultaneously on the RVE model.

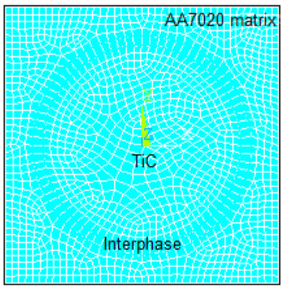

Figure 1: The RVE model

3. Results and Discussion

The finite element analysis (FEA) was carried out at -300°C to 400°C temperature conditions. The hydrostatic pressure load was applied RVE model to investigate thermo-elastic tensile behavior of AA7020/TiC nanoparticulate composites. The volume fractions of SiO_2 nanopaticles in the AA7020 matrix were 20% and 30%.

3.1 Thermo-elastic behavior

Elastic and thermo-elastic strains as a function of temperature are showed in figure 2 and 3. The elastic and thermo-elastic strains increased with increase of temperature except above 200°C for the composites having volume fraction of 20% TiC. The regression fitness of elastic strain into linear equation is as follows:

For 20% TiC, elastic strain = $5\times10^{-6}T - 0.009$ (1)

For 30% TiC, elastic strain = $6\times10^{-6}T - 0.016$ (2)

The regression fitness of thermo-elastic strain into linear equation is as follows:

For 20% TiC, thermo-elastic strain = $3\times10^{-5}T - 0.009$ (3)

For 30% TiC, thermo-elastic strain = $1\times10^{-5}T - 0.016$ (4)

R-squared is a statistical measure of how close the data are to the fitted regression line. In general, the higher the R-squared, the better the model fits the data. The R-squared values of elastic strains are, respectively, 0.407 and 0.994 for 20%TiC and 30% TiC composites. . The R-squared values of thermo-elastic strains are, respectively, 0.956 and 0.999 for 20%TiC and 30% TiC composites. For composites with high volume fraction (30%) of TiC, the elasto-compressive strain was higher than that for low volume fraction (20%) of TiC. The basic reason could be the mismatch of CTE between AA7020 alloy and TiC.

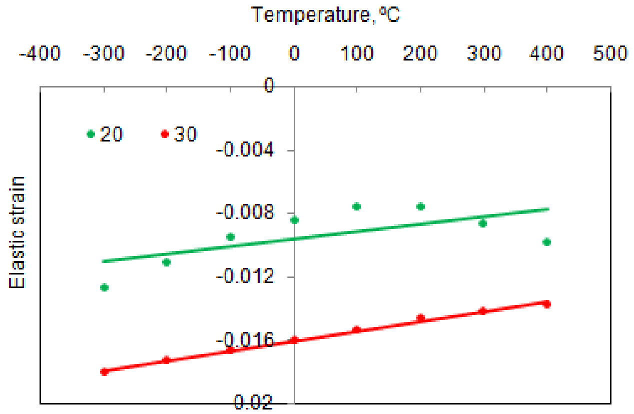

Figure 2: Influence of temperature on elastic strain.

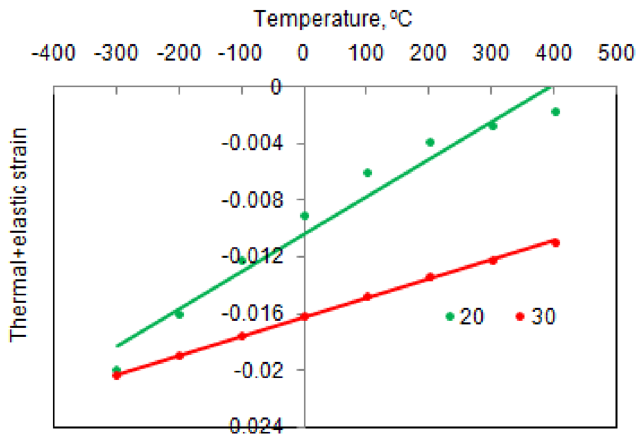

Figure 3: Influence of temperature on thermo-elastic strain.

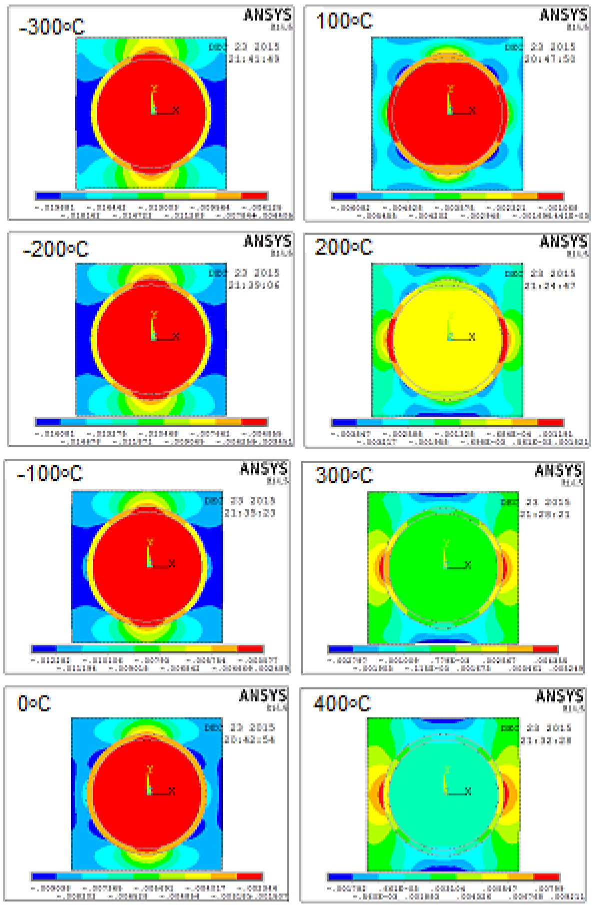

Figure 4: Raster images of thermo-elastic strain of AA7020/20% TiC composites.

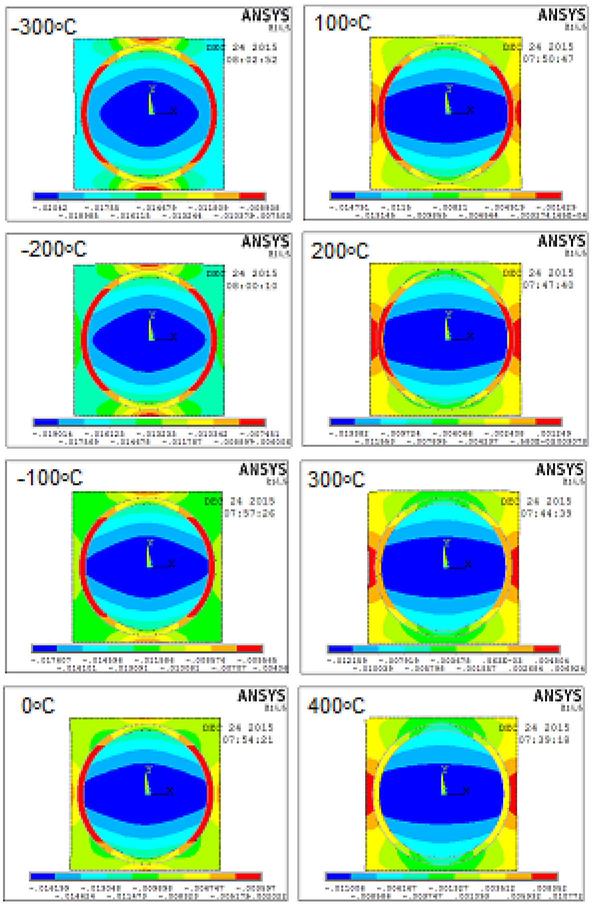

Figure 5: Raster images of thermo-elastic strain of AA7020/20% TiC composites.

The composites having low volume fraction (20%) of TiC nanoparticles experienced the tensile strains (red color) as the temperature changed from -300°C to 100°C temperature while the AA7020 alloy matrix experienced the compressive strains as shown in figure 4. Above 100°C the interphase only experienced the tensile strains; the matrix and TiC nanoparticle experienced the compressive strains. The composites having high volume fraction (30%) of TiC nanoparticles experienced the compressive strains as the temperature changed from -300°C to 0°C while the interphase and AA7020 matrix alloy experienced the tensile strains (red color) as shown in figure 5.

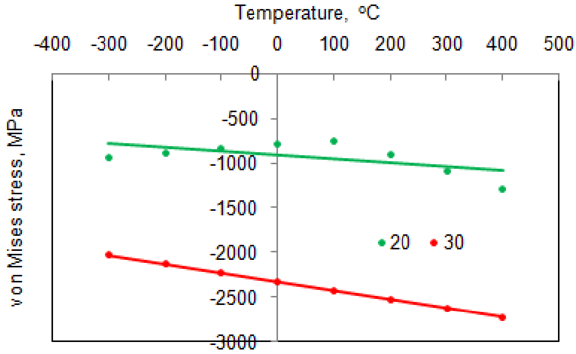

Figure 6: Influence of temperature on tensile strength.

Compressive strength as a function of temperature is depicted in figure 6. The compressive strength deteriorated with the increase of temperature. The compressive strength escalated with the increase of volume fraction of TiC. The stiffness (elastic modulus) increased with the increase of temperature (figure 7) of AA7020/TiC nanoparticulate composites. The stiffness was raised steeply above 100°C for low volume fractioned (20%) TiC composites. This is very interesting phenomena to be scientifically explored. The probable reasons as per my knowledge might be as follows:

- A higher modulus in general indicates that the material is harder to deform [20]. This indicates that the AA7020 matrix was no longer to carry hydrostatic and thermal loads. Because of load transferred from matrix to TiC nanoparticles, very large hydrostatic force was required for small deformation of TiC. The Brinell hardness numbers of TiC and AA7020 alloy are, respectively, 2400 and 105.
- When the temperature increases, the atomic thermal vibrations increase, and this causes the changes of lattice potential energy and curvature of the potential energy curve. Hence, the elastic modulus changes with temperature.
- The change of elastic modulus with temperature involves two characteristics: the atomic binding force and the volume of material. The bulk modulus of a material is dependent on the form of its lattice, its behavior under expansion and the vibrations of the molecules. These characteristics are reliant on temperature.
- The bulk modulus is a thermodynamic quantity. To specify bulk modulus, it is necessary to state how the temperature varies during compression: constant temperature (isothermal) and constant entropy (isentropic). In the present work, it is isothermal. For that reason, the bulk modulus is directly proportional to applied pressure.
- According to the third law of thermodynamics, the derivative of any elastic constant with respect to temperature must approach zero as the temperature approaches absolute zero.

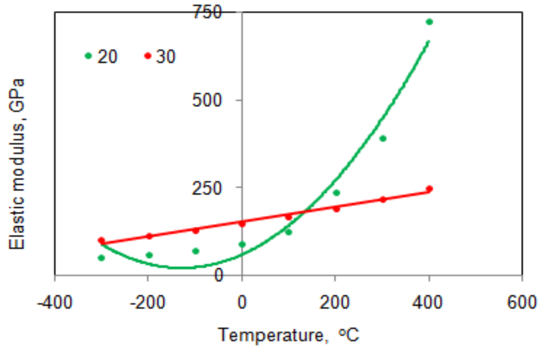

Figure 7: Influence of temperature on elastic modulus.

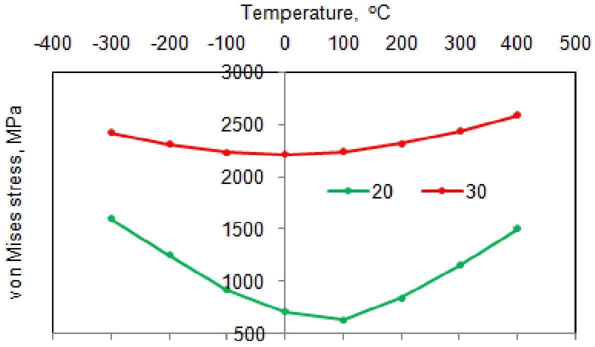

Figure 8: Influence of temperature on von Mises stress.

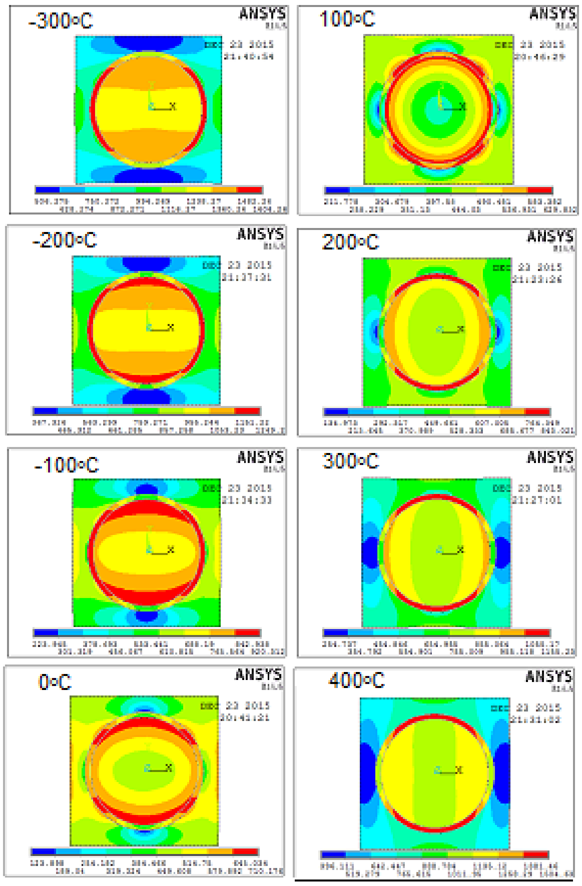

Figure 9: Raster images von Mises stress of AA7020/20% TiC composites.

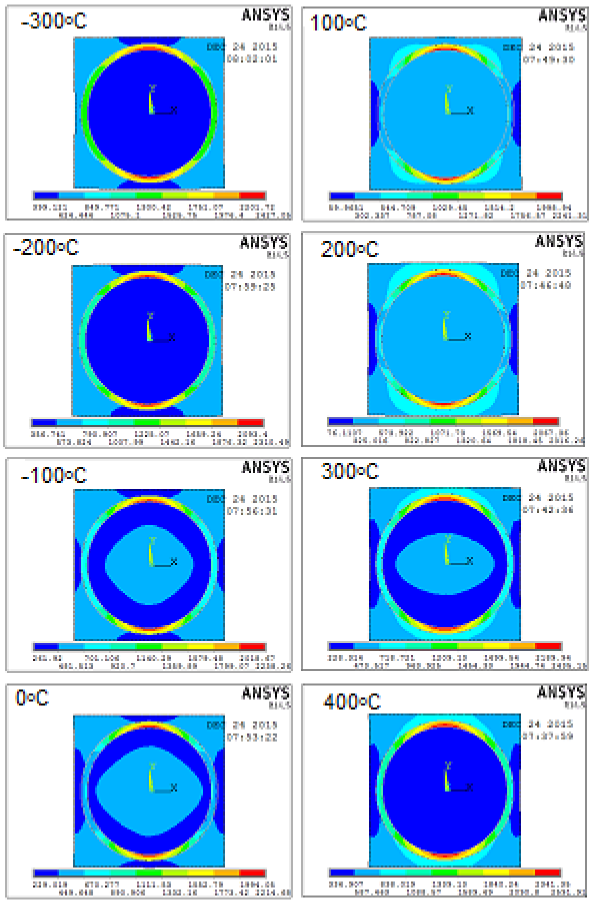

Figure 10: Raster images of von Mises stress of AA7020/30% TiC composites.

3.2 Fracture behavior

Figure 8 describes the von Mises stress induced in the composites. The von Mises stress decreased with the increase of temperature from -300^{o}C to 0^{o}C and later it increased with the increase of temperature. The von Mises stress was higher in the composites having 30% TiC nanoparticles than that in the composites consisting of 20% TiC. In all composites (figure 9 and 10), the interphase was fractured.

4. Conclusions

The elastic and thermoelastic strains increased with the increase of temperature. The compressive strength decreased with the increase of temperature. Interestingly, the stiffness increased with increase of temperature for AA7020/TiC nanoparticulate metal matrix composites. This might be the reason; TiC is being used as a heat shield coating for atmospheric reentry of spacecrafts.

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