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MICROSTRUCTURE REFINEMENT BY METALLIC PARTICLE IMPACT

[1] Vincent Lemiale, [2] Yuri Estrin, [3] Robert O'Donnell, [4] Hyoung Seop Kim

Grain refinement by plastic deformation is becoming increasingly popular as a way of producing metals with improved properties, such as higher mechanical strength. Surface treatment techniques in which a metallic substrate is bombarded with metallic particles can generate nanocrystalline layers in the impact zone. Understanding the physical mechanisms behind this grain refinement is crucial to achieve an improvement of existing experimental processes. In this paper, we propose a numerical framework combining finite element simulations with a dislocation-based material model to predict the evolution of the microstructure under particle impact. A single particle impacting a metallic substrate along its normal was simulated for different initial velocities. The simulations were compared with previously reported numerical and experimental data. The results indicate that our model accurately captures the grain refinement in the impact zone for a broad range of velocities. This approach provides valuable information on the formation of nanocrystalline layers in both the substrate and the impacting particle. It has potential applications in any process involving surface treatment by high-velocity particles, such as shot peening, surface mechanical attrition treatment, kinetic metallization, cold spray, etc.

Particle impact, grain refinement, finite element simulations, copper

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[1], [2], [3] CSIRO Division of Process Science and Engineering, Australia
[1] School of Mathematical Sciences, Monash University, Australia
[2] ARC Centre for Design in Light Metals, Department of Materials Engineering, Monash University, Australia
[4] Department of Materials Science and Engineering, Pohang University of Science and Technology, Korea

1. Introduction

It is well known that a number of mechanical properties in a polycrystalline metal are improved when its microstructure is refined. Most notably, fine grained metals are usually much stronger than conventional coarse grained ones. The way to ultra fine grain structures in metals and alloys with sufficiently large stacking fault energy may be via severe plastic deformation, which results in the formation of dislocation cell structure and its transformation to a refined grain structure.
A number of surface treatment techniques are based on this concept. For instance, in shot peening, the surface structure is modified through a series of impacts by steel balls imparted on a sample. In some cases, it has been shown that nanocrystalline layers (with an average grain size less than 100 nm) could be obtained at the interface between a particle and the substrate [1, 2]. To enhance our ability to fabricate homogeneous fine grained layers, it is essential to gain a better understanding of their formation under individual particle impacts. In this context, the use of numerical techniques such as finite element (FE) analysis may provide an insight into the details of mechanical behavior under high-speed deformation, which in many cases cannot be captured experimentally. This, however, is only possible if an adequate constitutive description based on microstructure evolution is used in an FE simulation.
A number of numerical models of particle impact were reported in literature. These simulations were able to cover the observed deformation pattern for a vast range of initial velocity conditions [3-5]. However, most previous studies were focused on reproducing the material behavior at a macroscopic level, without accounting for the evolution of the underlying microstructure. Therefore, it was not possible with these models to estimate the characteristic length scale of the microstructure produced.
Recently, a dislocation-based model has been successfully applied to dynamic Taylor impact tests [6]. The model, originally developed in the context of severe plastic deformation processes operated at relatively low to moderate strain rates, was calibrated in [6] for pure copper deformed at high strain rates. A particular strength of this model lies in its ability to predict the evolution of the dislocation cell structure often observed in heavily deformed metals.
In the present paper, finite element analysis incorporating this material model, which was demonstrated to be adequate for high strain rate regime [6], is carried out to investigate the mechanical behavior of a single copper particle impacting on a copper substrate. The central aim of this work is to demonstrate that such an approach provides a potent tool for predicting grain size refinement induced by particle impact. For the velocity range investigated in this study it is shown that our approach correctly reproduces the observed experimental results reported in literature.

2. Numerical framework

2.1 Material model

In metallic materials with sufficiently high stacking-fault energy dislocation cells may form as a result of deformation to large strains. Experimental evidence of dislocation

cell formation under particle impact has been reported in literature [7]. It is therefore reasonable to assume that the constitutive model for dislocation-cell forming materials [8, 9] is applicable for such materials, at least in the region near the impacted surface. In the mentioned model, a material is considered as a two-phase one, composed of cell interiors containing a low dislocation density and cell walls with a high dislocation density. The model has been presented in detail in earlier papers [8-11], and therefore only its salient features relevant to the present study will be discussed here. The total dislocation density ρ_{tot} is calculated from the dislocation density ρ_w in the cell walls and the dislocation density ρ_c in the cell interiors. Taking into account the various physical mechanisms that take place at the dislocation level, the evolution of ρ_w and ρ_c can be described by the following set of differential equations [8]:

$$\dot{\rho}_c = \alpha^* \frac{1}{\sqrt{3}} \frac{\sqrt{\rho_w}}{b} \dot{\gamma}^r - \beta^* \frac{6\dot{\gamma}^r}{bd(1-f)^{1/3}} - k_0 \left(\frac{\dot{\gamma}^r}{\dot{\gamma}_0} \right)^{-1/n} \dot{\gamma}^r \rho_c \quad (1)$$

$$\dot{\rho}_w = \frac{\sqrt{3}\beta^* \dot{\gamma}^r (1-f)\sqrt{\rho_w}}{f\, b} + \frac{6\beta^* \dot{\gamma}^r (1-f)^{2/3}}{b\, d\, f} - k_0 \left(\frac{\dot{\gamma}^r}{\dot{\gamma}_0} \right)^{-1/n} \dot{\gamma}^r \rho_w \quad (2)$$

In these equations, b is the magnitude of the Burgers vector, f is the volume fraction of the cell walls, d is the cell size. $\dot{\gamma}^r$ is the resolved shear strain rate, while $\dot{\gamma}_0$ is a reference shear rate; n is a parameter inverse in the strain rate sensitivity of the dynamic recovery terms. Finally, α^*, β^* and k_0 are numerical constants.

The physical meaning of each of the terms in these equations can be found in [8]. For the clarity of this paper, it is only important to recall that they incorporate both dislocation generation/storage and annihilation mechanisms. Generation of dislocations is assumed to occur through the activation of Frank-Read sources within cell walls. Cross slip or climb mechanisms responsible for dislocation annihilation (dynamic recovery) are incorporated in the last term in Eqs. (1) and (2).

Once the cell wall and cell interior dislocation densities are known, the total dislocation density can be obtained from the following rule of mixtures:

$$\rho_{tot} = f\rho_w + (1-f)\rho_c \quad (3)$$

The average cell size is given by a scaling relation [8, 9]:

$$d = \frac{K}{\sqrt{\rho_{tot}}} \quad (4)$$

Usually, it is tacitly assumed in the models based on Refs. [8, 9] that for large strains giving rise to accumulation of misorientations between neighbouring dislocation cells, cell boundaries are gradually converted to large-angle grain boundaries. In other words, the calculated final cell-size is identified with the average grain size of the new structure. This model has recently been successfully applied to dynamic Taylor impact tests [6]. In the simulations of the Taylor test, the material parameters α^*, β^* and k_0 were calibrated using pure copper specimens subjected to high strain rates loading as a “gauge”. The results of this calibration can now be applied to the simulation of particle impact. In the present simulations, pure copper processed by two passes of equal-channel angular pressing (ECAP) described in Ref. [6] was selected. Therefore, the initial – very fine - microstructure was taken to be identical to that considered in [6]. In particular, the initial dislocation cell size d was set at 238 nm. All material parameters that appear in Eqs. (1)-(4) were also reported in [6].

2.2 FE model

The finite element package employed in the present work was MSC-Marc [12]. A single copper particle impacting on a copper substrate normally was considered, therefore only a 2D axisymmetric model was necessary. For impact analysis, it is common to use an explicit algorithm to integrate the equations of motion. However, a preliminary study of the software capability has led to the choice of an implicit single step Houbolt algorithm [13]. While this choice has an effect on the computation time, other studies on dynamic impact suggest that this algorithm produces results similar to a direct explicit integration [14].

A four-node element with full integration scheme was chosen. In addition, a special 'constant dilatation' formulation was selected to prevent volume locking known to occur for large deformation [13]. This formulation was preferred over a reduced integration scheme as spurious deformation modes were observed when it was employed in our simulations even when hourglass control was used.

In most simulations, the initial mesh size in the vicinity of the particle substrate interface was set at 0.5 μm and 0.6 μm for the particle and substrate, respectively. This is about twice the size of the initial grain size. Since our constitutive model incorporates information at the microstructure level, it is important to ensure that the average element size is not smaller than the average grain size. Indeed, in discretizing a domain into a finite element mesh and applying a constitutive model, it is tacitly assumed that a continuum description is adequate for each element. If the element size is smaller than the average grain size, this assumption may be questionable.

Due to the large strain occurring during impact, the finite element mesh may become distorted too much in the course of straining. This problem can be overcome by the use of a remeshing scheme. However, our simulations suggested that the remeshing scheme significantly influenced the solution, leading at the highest speeds to an unphysical deformed shape, as previously reported by others [3]. Consequently, no remeshing was used in the present study. The authors of [5] questioned the validity of the results obtained without remeshing by pointing out that the shear instability observed by some authors could be due to an excessive element distortion. However, our results did not indicate the appearance of shear instability, nor did they show a strong dependence on finite element mesh size. It was therefore concluded that the element distortion in the vicinity of the particle/substrate interface did not affect the results in any critical way.

The FE model setup including the initial mesh is shown in Figure 1. Also shown in this figure are the locations of the two nodes chosen for outputting purposes.

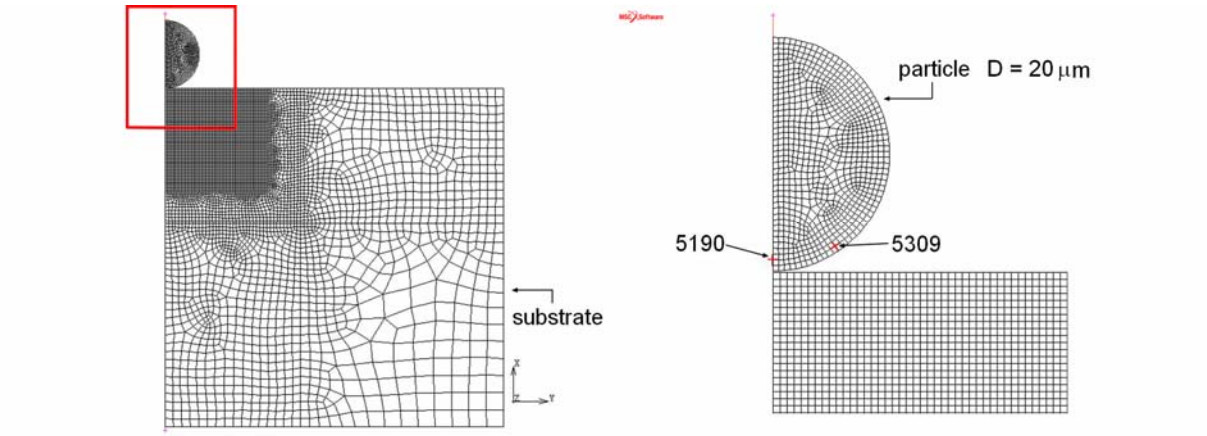

Figure 1. Geometry of the particle impact test considered in this work. The initial dimensions of the substrate are 100 μm x 100 μm. Symmetric boundary conditions are applied on the left edge of the model, while the bottom edge of the substrate is fixed. Also indicated are the locations of the nodes chosen for outputting purposes.

The model dimensions are similar to those for cold spray conditions [3, 4] so that a direct comparison with previous studies is possible. It has been determined that the critical impact velocity above which bonding between particle and substrate occurs in copper is about 500 m/s [15], although it should be noted that this value is not universally accepted [5]. The material under consideration in the present study was processed by two passes of ECAP, therefore it is expected that the critical velocity may be different to that for conventional coarse-grained copper.
The regime of interest for cold spray applications is obviously above this limit. However, for grain refinement investigation, it is also relevant to analyze the evolution of the microstructure at lower velocities. Therefore in the present study a range of velocities was investigated: from low (100-200 m/s) to intermediate (300-400 m/s) to high (500 m/s and higher) velocities.
It is important to note that our model as it stands does not incorporate a description of bonding possible in the latter velocity range. Also, physical mechanisms known to occur at extremely large strain rates, such as twinning, dynamic recrystallization or viscous drag of dislocations (instead of thermally activated dislocation glide), are not accounted for in our model. Therefore, predictions of the grain refinement made at the highest speeds are likely to be quantitatively imprecise. It should be noted that the use of empirical models, such as the aforementioned Johnson-Cook model, calibrated for a lower velocity range, suffers from the same limitations with regard to the highest strain rate encountered in cold-spray like conditions.
Finally, friction between the impacting particle and the substrate was included by means of a simple Coulomb model, with a representative value of 0.2 for the friction coefficient. Friction heat was included for impact velocities of up to 400 m/s, however this effect was ‘turned off’ at higher velocities. Indeed at the highest speeds sticking conditions between particle and substrate had to be enforced in order to prevent numerical errors due to contact. No significant difference with the case when friction heat was considered was found, which is consistent with the fact that at higher strain rates the solution will be dominated by heat generation due to dissipated work of plastic deformation.

2.3 Thermo-mechanical coupling

Thermo-mechanical coupling was included by setting the strain rate sensitivity exponents entering the model [8, 9] as being inversely proportional to the temperature, as explained in [6]. The fraction χ of plastic deformation dissipated as heat was assumed to be 90%. Heat conduction was included in the model, since it cannot be neglected in our case. Free heat transfer was assumed at the interface between particle and substrate. Finally, frictional heat was also included in the lower velocity range, as explained in the previous section.
The initial thermal conditions as well as thermal properties are given in Table 1. The density of copper was taken to be 8960 kg·m^{-3}.

T_{room} (K)	C_v (J·kg^{-1}K^{-1})	χ	λ ($W \cdot m^{-1} \cdot K^{-1}$)
298	385	0.9	400

Table 1. Initial temperature and the thermal parameters for pure copper.

3 Results and discussion

3.1 Deformed shape and overall mechanical behaviour

Figure 2 shows the equivalent (von Mises) plastic strain immediately after the kinetic energy of the system has reached its minimum, for various impact velocities. Three different modes of deformation have been identified. At the lower velocity, most of the deformation occurs within the particle, in a band starting at the particle/substrate interface and propagating into the particle. In the intermediate velocity range, the deformation is localized at the interface between the particle and the substrate, but – unlike in the highest velocity case - no 'jetting' is observed. At the highest velocities, a jet characteristic of the case of high-speed deformation is seen to form. The highly localized deformation at the highest velocity is due to the combination of dynamic inertia effect and local heating effect.
All of these qualitative observations are consistent with previously reported data [3, 5].

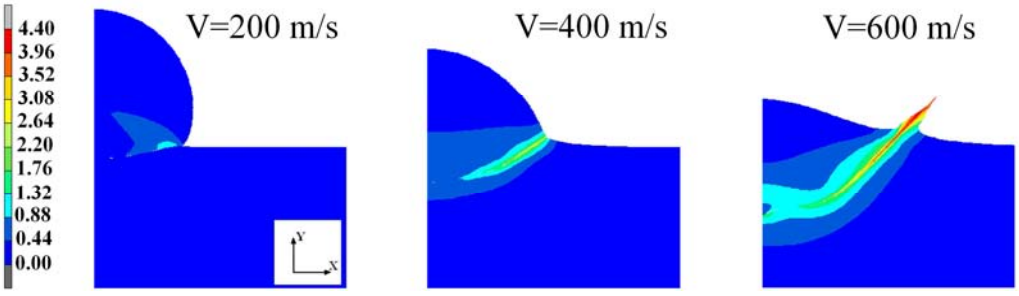

Figure 2. Equivalent plastic strain at the instant t corresponding to the minimum of kinetic energy for three different initial velocities representative of the three velocity range discussed in the text. Simulation time: t=38 ns, t=35 ns, t=38 ns.

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3.2 Evolution of dislocation cell size

A new element, which makes our model to stand out from most of the particle impact models, is its capacity to predict the microstructure evolution. Figure 3 displays the dislocation cell size distribution at the same instant as in Figure 2. The layer of most refined cell structure (tantamount to refined *grain* structure, see above) tends to be located at the particle/substrate interface. However, it is interesting to note that a reasonably large area of homogeneous refined material is predicted in our simulations. This is in agreement with what was described in our previous work [6]. This can be explained by the fact that a near saturation value of the cell size was reached in a relatively large region near the interface.

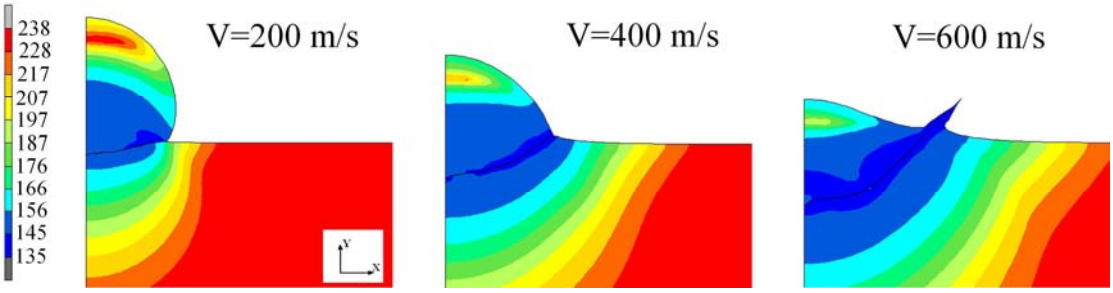

Figure 3. Cell size distribution (in nm) at the minimum of kinetic energy for three different initial velocities. Simulation time (from left to right): t=38 ns, t=35 ns, t=38 ns.

In addition to the spatial distribution of the cell size presented in Fig. 3, Figure 4 shows its temporal evolution as recorded near the interface, as well as the impact velocity dependence of the minimum cell size produced. The cell size drops precipitously immediately after the impact. The rate of cell size reduction then decreases, and after about 10-20 ns a near-saturation value is reached. It should be noted that, similarly to our previously reported results [6], an increase of the dislocation cell size after the initial microstructure refinement is observed in some cases, as can be seen in Figure 4. This can be attributed to the growth of the dynamic recovery terms in Eqs. (1) and (2) with temperature which in turn leads to a lower rate of dislocation accumulation in the region experiencing the greatest increase of temperature. This behaviour results in a saturation value for the final cell size with an increase of the initial velocity, as shown by the right curve of Figure 4. While our model predicts a minimum achievable cell size of about 135 nm, recently published results were reported with cell sizes below 100 nm [2]. The small discrepancy between our predictions and the experimental data can be explained by the fact that our model as it stands does not incorporate a number of physical mechanisms that are likely to influence the microstructure evolution. This will be discussed in more detail in a later part of the paper.

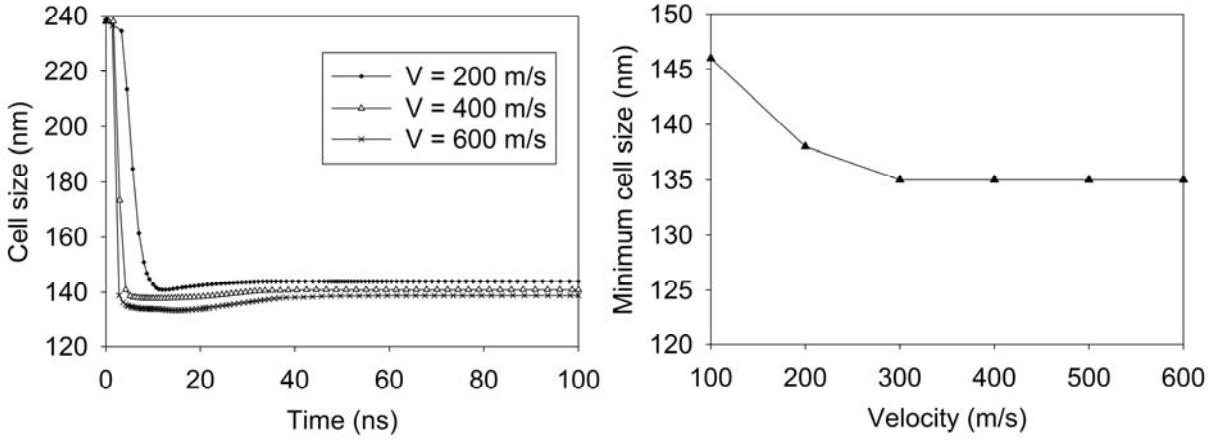

Figure 4. Cell size evolution during impact as recorded at node 5309 (see Figure 1).

3.3 Stress calculations

The evolution of the equivalent von Mises stress as recorded near the particle/substrate interface is presented in Figure 5. Also shown on this figure is the maximum pressure at the interface as a function of the initial velocity of the particle.

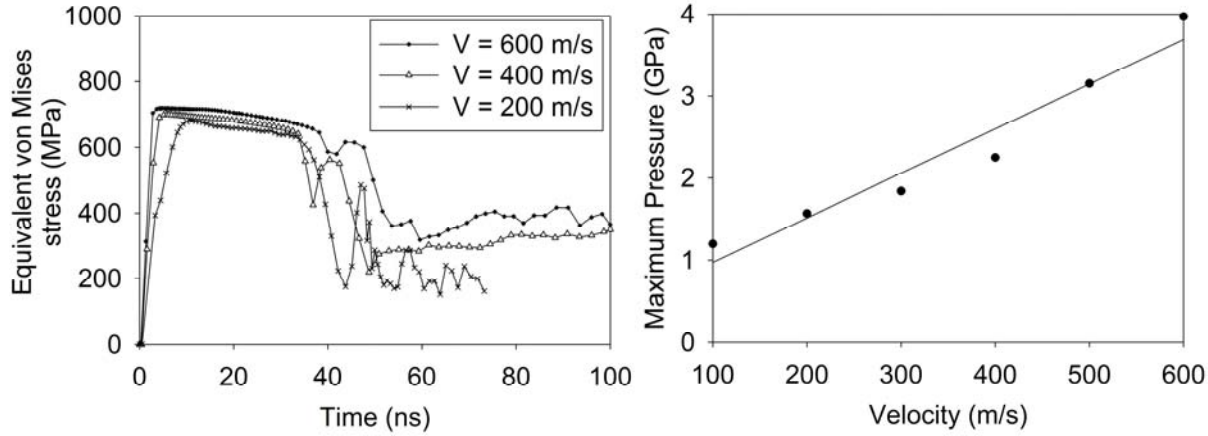

Figure 5. Left: evolution of equivalent von Mises stress with time at three different velocities, as recorded at node 5309 (see Figure 1). Right: maximum pressure reached at node 5190 (see Figure 1) as a function of impact velocity.

Very high stress levels are reached under high stain rates. This is supported by recent experimental tests performed on nanocrystalline copper at high strain rates [16]. Consistent with the saturation value of the minimum attainable cell size observed in our simulations and discussed in the previous section, a saturation of stress was observed as the initial velocity was increased. Unlike earlier results [3], no adiabatic shear localization was apparent in our simulations. This difference may be explained by the fact that the adiabatic conditions assumed by the authors of [3] tend to promoted strain localization. An alternative explanation may be that thermo-mechanical coupling included in the present work through the temperature

dependence of the strain rate exponents is not strong enough to give rise to strain localization.

3.4 Temperature distribution

The temperature evolution near the particle/substrate interface and the dependence of the maximum temperature on the initial particle velocity are shown in Figure 6.

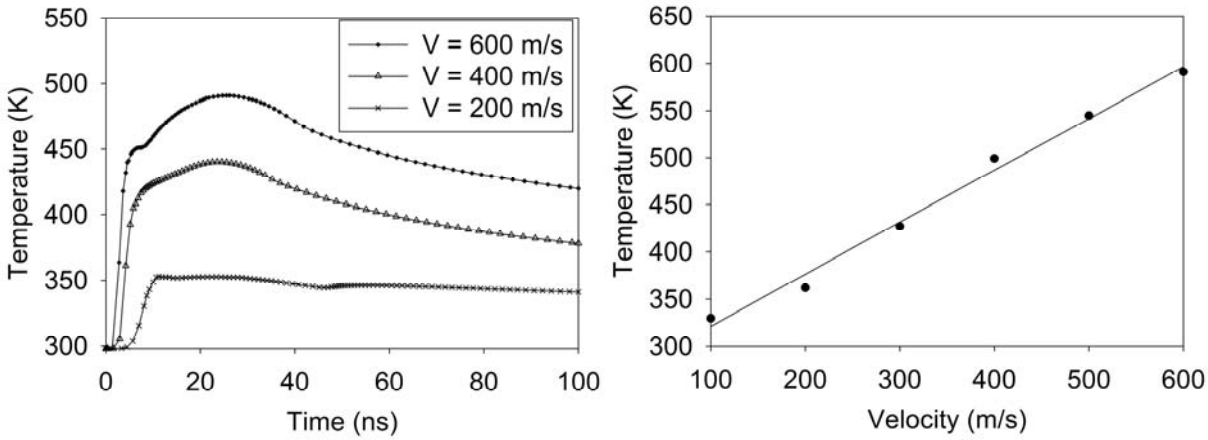

Figure 6. Left: temperature evolution as recorded at node 5309 (see Figure 1) at three different velocities. Right: maximum recorded temperature as a function of the initial particle velocity.

As seen from Figure 6, there is a sharp increase of temperature in the first 10-20 ns of impact, especially at the highest particle velocity. Nevertheless, it should be noted that in all our simulations where heat conduction was included, the predicted maximum temperature was well below the melting temperature for copper. Our results indicated that the adiabatic assumption commonly adopted in the literature under similar impact conditions is not justified here. Indeed, the maximum predicted temperature is largely overestimated when making this assumption, which explains the observed difference between the present results and previously reported numerical results [3, 4].

4 Conclusion

Structure refinement of polycrystalline metals (exemplified by ultrafine grained copper) under high strain rate impact conditions was investigated by means of finite element analysis. Simulations of a copper particle impacting on a copper substrate showed that extreme grain refinement occurs near the interface between the two bodies, in reasonably good agreement with available experimental data. Moreover, for the velocity range investigated three different regimes were identified, which was also consistent with previously published results. It is therefore concluded that the numerical framework used in this study together with a dislocation-based model suitable for describing severely deformed materials can be used to analyze grain size refinement under impact conditions.

However, our model in its present form is limited to a velocity range for which the induced strain rates do not exceed about 10^4 s^{-1}. At higher velocities, a number of physical mechanisms are known to become preponderant in copper, which however were not included in the model. The most critical ones are deformation twinning, dynamic recrystallization and viscous drag of dislocations (rather than their thermally activated glide) in the high velocity regime. Furthermore, at the high end of the impact velocity range (such as in cold spray), metallic bonding between particle and substrate would take place and this process is not accounted for in the model. Still, the model was demonstrated to provide a useful tool for predicting the deformation behavior and microstructure evolution of the impacting particle and the substrate in a broad range of conditions. Used in conjunction with experiments, this numerical tool can significantly improve our current understanding of the microstructure evolution in metallic materials under impact conditions.

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[1], [2], [3] CSIRO Division of Process Science and Engineering, Australia
[1] School of Mathematical Sciences, Monash University, Australia
[2] ARC Centre for Design in Light Metals, Department of Materials Engineering, Monash University, Australia
[4] Department of Materials Science and Engineering, Pohang University of Science and Technology, Korea