NON-EQUILIBRIUM PHENOMENA IN METALS AT HIGH STRAIN RATES

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ABSTRACT

Metals and other materials subjected to non-equilibrium thermodynamic stimuli may incur irreversible and remarkably well-structured damages. In stressed metals, slip bands and dislocation cells are the defects of our interest. The query here is not so much whether the microstructural arrangement occurs. We know that it does. Our interest is in answering a more fundamental question, namely what are the mechanisms which necessitate the reconfiguration. Prigogine [1] stated that the secret to the system's survivability with its microstructural integrity intact is in an exchange of energy. A stable complex system receives low-entropy energy from the environment while giving away energy that is entropy rich. A metal subjected to extreme strain rates $(10^3/\text{sec and})$ above) becomes such a thermodynamically open system characterized by the flux of energy due to the high mobility of dislocations [2]. In stressed crystals, there is a synergetic interaction between the redistribution of energy and the formation of slip bands and other defects. Consequently, the defects are reshuffled into well-spaced domains and cause that a portion of internal energy is stored, while a locally negative rate of entropy become a probable outcome. One could forecast many such processes of the energy redistribution but only some of them pave the way towards the state of steadiness and equilibrium. The intent of the development is to predict an optimal arrangement of the stress induced defects. The optimal configuration provides the stressed material with the opportunity to minimize the damage and, in this manner, brings it as close to the thermodynamic equilibrium as possible.

In the proposed approach [3], we utilize the well-known concept of steadiness and further expand it into the more complex behavior relevant at extreme loading rate. Typically, the steady behavior is described in terms of a path $\zeta_k^{steady} = x_k - \upsilon_k^{\varsigma} t$, where state variables (such as internal energy, entropy, etc.) remain unchanged at fixed positions along ζ_k^{steady} . This also means that an observer placed at the point x_k and moving with constant velocity υ_k^{ς} does not detect any changes in the surroundings. We hypothesize that in a material subjected to complex loading there is a non-steady path $\zeta_k = \zeta_k(x_l, t)$ such that at each position along the path entropy, energy and temperature are constants. In other words, the thermodynamic variables are expressed

entirely in terms of the path ς_k . In this construction, the non-steady path evolves during the thermodynamic process. The complex behavior can be brought into the state of steadiness (the path evolution is complete) and equilibrium, where there is no further exchange of energy. There are instances when the state variables (energy, entropy and temperature) exhibit discontinuous responses. Hence, the non-steady path breaks down and higher order arrangements emerge.

First, we invoke several experimental observations, which together, challenge our understanding of the dynamic behavior of metals. The challenges set the foundation for the development of the theoretical approach, which includes a continuum level description of the stress induced defects and offers thermodynamics based justifications for the defect self-organization We apply the theory to the classic problem of a shocked metal at uniaxial strain condition and show that the theory is capable of explaining the seemingly disconnected phenomena discussed in the introductory part of the presentation. The approach has been tested for copper with the use of large 3-D simulations of a spherical shell either subjected to a constant compressive stress or tension. The analysis explains the formation of shear bands and the development of hot spots in the rapidly deformed material.

REFERENCES

- [1] I. Progogine, *Nobel Prize in Chemistry*, Royal Academy of Sweden, 1977.
- [2] A. Zubelewicz, et. al. Phys. Rev. B 71, 104107, 2005.
- [3] A. Zubelewicz, *Phys. Rev. B*, submitted for publication.