IMPACT METAMORPHISM: ON THE WIDTH OF THE GAP BETWEEN OBSERVATION AND MODELING – THE GEOLOGIST'S VIEW VS. THE MODELERS ASSESSMENT I. K. Wünnemann[1], A. Deutsch[2], [1]Museum für Naturkunde, Humboldt-Universität, Invalidenstraße 43, Berlin 10099, Germany, kai.wuennemann@museum.hu-berlin.de, [2]Institut für Planetologie, WWU Münster, Wilhelm-Klemm-Str. 10, Münster 48149, Germany, deutsca@uni-muenster.de.

Introduction: Impact induced shock waves create distinctive imprints on minerals and rocks, summarized under the term *impact(shock) metamorphism*. Depending on the stress amplitude of the shock wave there is a progressive increase in the degree of shock deformation ranging from brittle damage (brecciation), the generation of shatter cones (fracturing), PDF development, solid-state high-pressure modifications (transformation), to whole rock melting and vaporization of rocks. The physics of shock waves and the resulting modifications in rocks and minerals have been investigated in great detail by experiments [1], observations at terrestrial impact craters [2], and in meteorites and lunar rocks. But only numerical modeling of shock compression and subsequent release can record the entire thermodynamic path the material is exposed to during the passage of a shock wave. Therefore, modeling is an absolutely essential tool complementing the study of shock wave propagation in solids, the design and interpretation of shock and cratering experiments, and the understanding of distribution of shock induced features in real impact craters.

Numerical models: Our understanding of the formation of shock-specific features in solids as a function of the pressure amplitude results primarily from sample recovery shock experiments and shock physics. Numerical models are in principle very similar to experimental techniques and can be understood as "numerical experiments", but without the technical limitations of experiments like restricted pressure ranges, short shock plateaux, or small sample size. In all numerical models the area of interest (single grain, rock unit, or large target area) is divided into small units (computational cells) of constant properties. Therefore, it is important to distinguish between models designed to explain processes on small (meso/micro) scales (e.g., mineral grains or pore space) and simulations at the scale of craters, in which computational cell sizes may reach tens or hundreds of meters. Micro- and meso-scale models provide information directly comparable to observations on field specimens or from experiments; crater models only compute the thermodynamic conditions that large (depending on cell size) rock units experience in the course of processes. Still, these results can be related to observations at natural impact structures. Generally it should be kept in mind that numerical models are only as good as our knowledge of the physics that govern the processes we are interested in. The main achievement of numerical modeling then lies in the simulation of the complex interplay of the various processes that can not be taken into account simultaneously in analytical approaches.

Modeling of shock features: Very few modeling studies have dealt with shock metamorphism itself (meso-scale models). Such models are analogous to shock experiments with the important advantage that the dynamic processes can be recorded. A good example is the modeling study of the formation of shatter cones by heterogeneities in rocks [3]. Any heterogeneity in rocks has a specific scale (mm to hundreds of m). Yet even "large-scale" heterogeneities are usually small at the scale of cratering models and can only be taken into account in meso/micro-scale models. Some studies are dealing with the behavior of shock waves along lithological interfaces, open cracks, and pores [4-6]. All models show that the lithological heterogeneities can explain the localized appearance of shock features (e.g., due to shearing along interfaces or closure of open cracks and pores). However, all models simplify the complex character of rocks.

Shock wave decay: On a larger scale (size of an impact crater), numerical models cannot provide the detailed information discussed above, but they can be used to compute the decay of the shock wave in the target as a function of distance, impactor parameters (velocity, size, and composition), and target properties (composition, strength, layering, porosity). Modeling the shock decay behavior in a given lithology depends critically on the equation of state (EOS), which relates the thermodynamic variables density, pressure, and internal energy. The computation of temperatures, however, is one of the weak points in hydrocode modeling so far. It should be noted also that models of shock wave decay are very sensitive to the resolution (number of computational cells); usually a large number of computational cells is required to provide good results. There are numerous modeling attempts for attenuation of shock waves in rocks [e.g. 7] but only recently has the effect of the very important property "porosity" been included in modeling [8]. The crushing of pore space is an effective mechanism for absorbing shock waves resulting in a much faster decay of the shock pressure and in much higher post-shock temperatures than observed in nonporous rocks (e.g., lunar agglutinates). Therefore, some shock features occur at lower shock pressures in porous materials than in competent rock [9,10].

The common approach to record the thermodynamic history of materials in numerical models is the usage of massless tracer particles. In this method, a tracer is placed into computational cells or along certain profiles of interest. While the tracers move through the computational grid, their thermodynamic path is recorded. The tracer's final position and the recorded peak shock pressure can then be compared with field observations, summarized as shock barometry on impact structures [1]. This approach is one of the most valuable linkages between nature and numerical modeling.

Melting and vaporization occur during or after release from shock wave compression when a certain material-dependent threshold pressure is exceeded (50 to >100 GPa in crystalline rocks, for whole melting [1]). As projectile velocity in impact experiments is insufficient to yield significant amounts of melt, the melt production in impact craters can only be investigated by hydrocode modeling. The generated melt volume is closely related to the understanding of shock wave decay or distribution of peak shock pressure in the target. Therefore, the above described tracer method can be used to derive the volume of impact melt. In earlier studies [7] lines of tracer particles were used to determine shape and size of the area where shock pressures exceed the critical pressure for melting. The volume of this area then corresponds to the melt volume produced in an impact event. It was found that melt and vapor production scales with the energy of the impactor [7] and that the region of melting is roughly spherical. This finding is in agreement with more recent studies, where a tracer was located in each computational cell [11]. The melt volume is then determined by summing up the corresponding volume of tracers (the volume of the cell that the tracer was initially located in) that experienced shock pressures in excess of the critical melt pressure [11]. For oblique impacts the shape of the melting region is assymmetric and the volume decreases by 20% for impacts from 90° to 45° [12]. In general, modeled melt volumes agree well with estimates based on observations at crater structures in crystalline targets [7]. But predictions have failed for craters in sedimentary or mixed targets [10]. Whether this is due to inappropriate treatment of porous and water saturated rocks in numerical models or whether there is actually much more melt present than detected so far [13] has remained unsolved. The recent drilling at Lake Bosumtwi revealed much less melt than predicted [14]. Yet in fact, craters in porous target materials should contain more melt due to the extra heat that is generated by the crushing of pores [10].

Damage: When the shock decays, with increasing distance from ground zero, below the HEL (Hugoniot elstic limit), only brittle fracturing and cataclasis occur in the rocks. In numerical models brittle deformation of the rocks is quantified by a damage parameter. Damage is a state variable included in many codes that describes the degree of fracturing; but as a scalar quantity it does not provide any information of fracture size, length, or direction. Damage covers micro-cracks as well as large fractures. Damage is accumulated due to tensile and shear failure, and both processes can be separated in numerical models [15]. Size and shape of the zone damaged by brittle fracturing are responsible for most geophysical anomalies observed at impact structures (gravity, seismics) [16]. However, models cannot provide any information about the increase of open pore space that is introduced by the opening of fractures (shear bulking or dilatancy). Quantification of this process would allow direct comparison of gravity anomalies with numerical models of crater structures.

Discussion: The progressive development of sophisticated codes has resulted in increasingly more realistic models of real collisions. Nevertheless the major shortcoming that will remain for the future is resolution: a km-scale impact model can not provide detailed information on the micro-scale but gives the thermodynamic conditions that larger rock units were exposed to. So, there will always be a distinction between meso/micro-scale models and studies that are aiming at crater formation as a whole. Other shortcomings include insufficiently accurate EOS, although. better constitutive models of geological materials can in principle be developed to result in major improvements in modeling.

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