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A microscale model for strain-induced phase transformations and chemical reactions under high pressure

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Abstract. – A simple strain-controlled kinetic equation for strain-induced phase transformations and chemical reactions is thermodynamically derived. This model is applied to explain various mechanochemical phenomena observed under compression and shear of materials in diamond or Bridgman anvils. In particular, it explains zero-pressure hysteresis and the appearance of new phases, especially strong phases, which were not obtained without shear. Also an explanation was obtained as to why a nonreacting matrix with a yield stress higher (lower) than that for reagents significantly accelerates (slows down) the reactions. Some methods to characterize and control strain-induced transformations and reactions are suggested.

Introduction. – Mechanochemistry studies the plastic strain-induced structural changes (SCs) which include phase transitions and chemical reactions. High-pressure mechanochemical phenomena are widespread in nature, physical experiments, and modern technologies. Mechanosynthesis (mechanical alloying), shear-induced amorphization, metallization and oxidation, shear ignition of energetic materials, interpretation of geophysical experiments (*e.g.*, deep earthquakes), and friction and wear data are proper examples. The most fundamental results in strain-induced SCs were obtained in rotating Bridgman or diamond anvils. After compression of the materials in Bridgman or diamond anvils, a very high pressure is produced in the specimen which leads to a number of SCs. It is known, from numerous experiments obtained in rotating Bridgman or diamond anvils [1–14] that the addition of plastic shear, due to the rotation of an anvil, leads to findings that have both fundamental and applied importance. 1) *Plastic shear leads to a significant (in some cases by a factor of* 3–5*) reduction of transformation* [2–4] *and reaction* [5,6] *pressure.* 2) *It also leads to the formation of new phases which were not produced without shear* [5–10], in particular, phase V of fullerene C_{60} [9,10] which is harder than diamond. 3) *The volume fraction of the new phase or the reaction product is an increasing function of the plastic shear strain* [2–6]. Therefore, strain-controlled (rather than time-controlled) kinetics is considered. 4) *Plastic shear reduces pressure hysteresis*, *i.e.* the difference between the start pressure of direct and reverse transformation [2–4, 11], in some cases to zero [11]. From this, it was claimed that the obtained transformation pressure can be interpreted as an equilibrium pressure. 5) In some cases, *shear deformation substitutes a reversible transformation with an irreversible transformation* [12]. Consequently, the rotation of an anvil allows the production of phases which are metastable at normal pressure and can be used in engineering applications. These results indicate that shear deformation increases pressure hysteresis, which is in contradiction with the previous statement.

Despite the fundamental and applied significance of the effect of plastic shear on SCs, there have only been our attempts to develop a corresponding theory at the macroscale [13, 14] (plastic flow of a sample with SC) and nanoscale [15, 16] (nucleation at a dislocation pile-up), as well as Gilman's [17, 18] qualitative atomistic model. None of them can explain most of the above phenomena. The fact that the above phenomena are observed for various transformations and reactions in various classes of materials suggests that there are some *universal microscopic (at the scale of* 1–1000 μm*) reasons for them which are independent of specific atomistic and nanoscale mechanisms of SC and material system.* The goal of this paper is to develop an approximate conceptual microscale approach, which allows the explanation of the above phenomena. A simple *strain-controlled kinetic equation* for strain-induced SC was thermodynamically derived, using the known phenomenology of strain-induced SCs [19, 20], our thermodynamic criterion for a thermal nucleation at the nanoscale [21, 22], and some results from nanoscale study [15, 16, 23]. An analysis of stationary solution of this equation allowed us to explain the above experimental phenomena. In addition, some methods to characterize and control strain-induced SCs were suggested. These methods can be used, in particular, to obtain and intensify SCs which were not obtained otherwise, *e.g.* leading to metallic hydrogen [24–26].

Summary of nanoscale model [15, 16]. – Pressure-induced SCs occur predominantly at existing defects, so a number of nucleation sites is limited. It is well known in steel research [19, 20] that strain-induced nucleation occurs at new defects generated during plastic flow. We assume that this is also true for SC under high pressure in any material. Stress concentration near the defects significantly increases the driving force for the SC and can cause SCs at significantly lower external pressure. It leads to barrierless nucleation, which does not require thermal fluctuations, and explains the strain-controlled rather than time-controlled kinetics. Indeed, the prescribed strain increment generates defects (dislocation pile-ups, shear-band intersections, grain and subgrain boundaries) with barrierless, *i.e.* very fast, nucleation and growth of the new phase up to the size where stress concentration is reduced and cannot drive the interface further. For the observation time of 1 s, this looks like an instantaneous SC. As straining stops, no new defects and nuclei appear, and the growth of the existing nuclei is thermodynamically impossible. As the contribution of the stress concentration to the driving force for SC is finite, there exists a lowest possible pressure, $p^{\mathrm{d}}_{\varepsilon}$, below which strain-induced SC is impossible. Defects generate both compressive and tensile pressures, which are of the same magnitude, *e.g.* for dislocation pile-ups. Consequently, they simultaneously promote both direct and reverse SC in different regions. All of these results will be conceptually incorporated in our microscale model. Moreover, for two-phase mixture 1+2, the stronger the phase 2 is, the smaller fraction of the plastic strain is concentrated in it. For chemical reactions, plastic flow produces a fragmentation and mixing of components similar to the liquid-phase reaction [5,6], so mixing will not be considered as the limiting factor. We believe that the above facts represent basic microscopic reasons for the mechanochemical phenomena considered in this paper.

Thermodynamically consistent strain-controlled kinetic equation for SC. – Let us consider a representative volume V consisting of a mixture of materials 1 and 2 which can transform to each other via SC (fig. 1). In the case of chemical reaction, both materials can consist of several substances. For brevity, we will use the terms phase 1 and 2. Plastic deformation of the volume V will be described in terms of equivalent plastic strain q (Odqvist parameter [27]) with values q_1 and q_2 in phases 1 and 2. Strain-induced SCs $1 \rightarrow 2$ in phase 1 and $2 \rightarrow 1$ in phase 2 occur simultaneously. Our goal is to derive the strain-controlled kinetic equation $\mathrm{d}c/\mathrm{d}q = f(p, c)$, where c is the volume fraction of phase 2 and p is the macroscopic pressure applied to V. Since time is not an explicit parameter, a kinetic equation has to be derived using the ther-

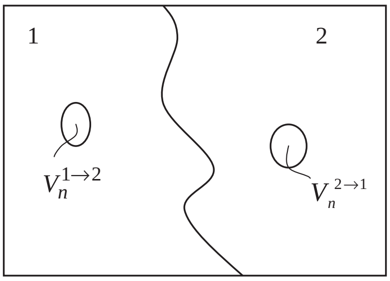

Fig. 1 – Representative volume V consisting of a mixture of phases 1 and 2. $V_n^{1\to 2}$ and $V_n^{2\to 1}$ are small volumes of phases 1 and 2 undergoing SC.

modynamic criterion (1) and an averaging procedure which is extremely complex. To obtain a simple analytical expression, we approximate the microscopic transformation work averaged over the transforming volume $V_n^{1\to 2}$ (fig. 1) by a decreasing function of $\mathrm{d}c/\mathrm{d}q_1$ (eq. (2)). The validity of such an approximation follows from our finite-element modeling [23]. Resolving the thermodynamic SC condition for $\mathrm{d}c/\mathrm{d}q_1$ (eq. (3)) we obtain a strain-controlled kinetic equation for SC $1 \to 2$. Repeating the same procedure for SC $2 \to 1$ and expressing q_1 and q_2 via q and the yield stresses σ_{y1} and σ_{y2} of phases 1 and 2 (eq. (4)), we obtain the final expression (5) for $\mathrm{d}c/\mathrm{d}q = f(p, c)$. An analysis of the stationary solution of eq. (5) (eq. (6)) allowed us to explain the experimental phenomena enumerated above and suggest some methods to control SCs.

For solid-solid SC, the transformation strain, $\boldsymbol{\varepsilon}_\mathrm{t}$, transforms a unit cell of the stress-free parent phase into a unit cell of the stress-free product phase. In the simplest case, when the temperature θ is fixed and homogeneous in a transforming volume and the change in elastic moduli is neglected, the criterion for barrierless (athermal) SC in the multiconnected volume V_n of elastoplastic material is [21, 22]

$$X = \frac{1}{V_n}\int_{V_n}\int_0^{\boldsymbol{\varepsilon}_{t2}} \boldsymbol{T}\boldsymbol{:}\,\mathrm{d}\boldsymbol{\varepsilon}_\mathrm{t}\,\mathrm{d}V_n - \Delta\psi(\theta) = p\varepsilon_0 + \frac{1}{V_n}\int_{V_n}\int_0^{\boldsymbol{\varepsilon}_{t2}} \tilde{\boldsymbol{T}}\boldsymbol{:}\,\mathrm{d}\boldsymbol{\varepsilon}_\mathrm{t}\,\mathrm{d}V_n - \Delta\psi(\theta) = K. \qquad (1)$$

Here X is the driving force for SC, which represents the calculated dissipation increment due to SC only (*i.e.* excluding plastic dissipation) during the entire transformation process, averaged over the transforming region; K is the actual dissipation due to SC related mostly to interface friction; $\boldsymbol{T}$ is the stress tensor; $\Delta\psi$ is the jump in the thermal part of the free energy; $\boldsymbol{T}\boldsymbol{:}\boldsymbol{\varepsilon}_\mathrm{t} = T_{ij}\varepsilon_\mathrm{t}^{ji}$ is the transformation work, ε_0 is the volumetric transformation strain, and the indices 1 and 2 denote the values before and after SC. For elastic materials, the expression for XV_n coincides with the change in Gibbs energy of the whole system [21]. To receive the second equality in eq. (1), we decompose stress, $\boldsymbol{T} = p\boldsymbol{I} + \tilde{\boldsymbol{T}}$, into a sum of the macroscopic pressure p, and the microscopic heterogeneous contribution, $\tilde{\boldsymbol{T}}$; $\boldsymbol{I}$ is the unit tensor. Since $V \gg V_n$, the variation of p is negligible during a small SC increment. Macroscopic shear stress is limited by the yield stress, which in the experiments under consideration is smaller, by a factor of 10–100, than p. Thus, it is neglected. To calculate the integral in eq. (1) for $\tilde{\boldsymbol{T}}$, the specific mechanism of strain-induced nucleation has to be known and then the corresponding boundary value problem has to be solved numerically. *E.g.*, the nucleation at the shear-band intersection in TRIP steel was investigated in our paper [23] using the SC criterion (1) and a finite-element solution. One of the results which can be extracted from this investigation is that the transformation work significantly decreases when $\mathrm{d}c/\mathrm{d}q$ grows. Qualitatively, this has to be the case for any mechanism of nucleation at strain-induced defects, *e.g.* at slip band and dislocation pile-up. To approximately take into account, in an averaged-over-V microscopic

SC criterion, the contribution of nanomechanisms of strain-induced nucleation, we substitute the integral with its approximate estimate:

$$X_\mathrm{d} = p\varepsilon_0 - \Delta\psi + \Delta X_\mathrm{d}\left(1 - \frac{a}{(1-c)^\zeta}\left(\frac{\mathrm{d}c}{\mathrm{d}q_1}\right)^\chi\right) = K_\mathrm{d}\,. \tag{2}$$

Here ΔX_d is the maximal microscopic contribution to the transformation work, subscripts d and r are for direct and reverse SCs, and a, χ and ζ are parameters. The factor $(1-c)^\zeta$ takes into account that SC $1 \to 2$ occurs in phase 1 only. Define the pressure p^d_h under which SC can occur under hydrostatic condition without a strain-induced contribution by the equation $p^\mathrm{d}_\mathrm{h}\varepsilon_0 - \Delta\psi = K_\mathrm{d}$, and the minimal pressure p^d_ε under which strain-induced SC can start with infinitesimal rate by equation $p^\mathrm{d}_\varepsilon\varepsilon_0 - \Delta\psi + \Delta X_\mathrm{d} = K_\mathrm{d}$. Then $\Delta X_\mathrm{d} = (p^\mathrm{d}_\mathrm{h} - p^\mathrm{d}_\varepsilon)\varepsilon_0$. Solving eq. (2) for $\mathrm{d}c/\mathrm{d}q_1$, one obtains a thermodynamically consistent strain-controlled kinetic equation

$$\left(\frac{\mathrm{d}c}{\mathrm{d}q_1}\right)^\chi = \frac{(1-c)^\zeta}{a}\,\frac{p - p^\mathrm{d}_\varepsilon}{p^\mathrm{d}_\mathrm{h} - p^\mathrm{d}_\varepsilon}\,. \tag{3}$$

If the right-hand side of eq. (3) is less than zero, we will take it as zero. Simultaneously, strain-induced $2 \to 1$ SC will occur in phase 2, which can be described by similar equations. To define q_1 and q_2 we assume $q_1/q_2 = (\sigma_{y2}/\sigma_{y1})^w$, and $q = (1-c)q_1 + cq_2$, wherefrom

$$q_1 = q\frac{\sigma^w_{y2}}{\sigma_y}\,; \qquad q_2 = q\frac{\sigma^w_{y1}}{\sigma_y}\,, \quad \sigma_y = c\sigma^w_{y1} + (1-c)\sigma^w_{y2}\,. \tag{4}$$

According to eq. (4), the stronger the phase is, the smaller fraction of the equivalent strain is concentrated in it; for $\sigma_{y1} = \sigma_{y2}$ one has $q_1 = q_2 = q$. As for $\sigma_{y2} = (4-10)\sigma_{y1}$, q_2 is negligible, we estimate parameter $w = (2\text{–}5)$. Adding algebraically the rates of direct and reverse SCs and taking into account eq. (4), one obtains the final kinetic equation

$$\frac{\mathrm{d}c}{\mathrm{d}q} = \frac{\sigma^w_{y2}}{\sigma_y}\left(\frac{(1-c)^\zeta}{a}\right)^{1/\chi}\left(\frac{p - p^\mathrm{d}_\varepsilon}{p^\mathrm{d}_\mathrm{h} - p^\mathrm{d}_\varepsilon}\right)^{1/\chi} - \frac{\sigma^w_{y1}}{\sigma_y}\left(\frac{c^k}{b}\right)^{1/m}\left(\frac{p^\mathrm{r}_\varepsilon - p}{p^\mathrm{r}_\varepsilon - p^\mathrm{r}_\mathrm{h}}\right)^{1/m}. \tag{5}$$

For the case $k/m = \zeta/\chi = g$, an analytical stationary solution of eq. (5) can be found

$$c_\mathrm{s} = \frac{\tilde{p}^\xi}{\tilde{p}^\xi + M(1-\tilde{p})^n} \quad \text{with}\; \tilde{p} = \frac{p - p^\mathrm{d}_\varepsilon}{p^\mathrm{r}_\varepsilon - p^\mathrm{d}_\varepsilon}\,; \quad M = \left(\frac{\sigma_{y1}}{\sigma_{y2}}\right)^{w/g}\frac{a^\xi}{b^n}\,\frac{\left(p^\mathrm{d}_\mathrm{h} - p^\mathrm{d}_\varepsilon\right)^\xi}{\left(p^\mathrm{r}_\varepsilon - p^\mathrm{r}_\mathrm{h}\right)^n}\left(p^\mathrm{r}_\varepsilon - p^\mathrm{d}_\varepsilon\right)^{(n-\xi)}, \tag{6}$$

$n = 1/k$, $\xi = 1/\zeta$. It follows from eq. (6) that for $p \to p^\mathrm{d}_\varepsilon$ (and for $p \le p^\mathrm{d}_\varepsilon$), one has $c_\mathrm{s} = 0$. For $p \to p^\mathrm{r}_\varepsilon$ (and for $p \ge p^\mathrm{r}_\varepsilon$), one obtains $c_\mathrm{s} = 1$. Between these two pressures, c_s varies from 0 to 1 and the shape of the $c_\mathrm{s}(\tilde{p})$ curve depends on material parameters, see fig. 2. If $M \to 0$ (*e.g.*, if the second phase is much stronger and/or $b^n/a^\xi \to 0$, *i.e.* kinetics of the reverse SC is suppressed, and/or $(p^\mathrm{d}_\mathrm{h} - p^\mathrm{d}_\varepsilon)^\xi/(p^\mathrm{r}_\varepsilon - p^\mathrm{r}_\mathrm{h})^n \to 0$), then $c_\mathrm{s} \to 1$. In the opposite case $M \to \infty$, $c_\mathrm{s} \to 0$. A number of conclusions can be made from our analysis.

1) SC is promoted by plastic deformation at a pressure above p^d_ε only. This explains a seeming contradiction formulated in [13], namely, why large plastic deformation during the compression of materials does not cause SC, while relatively small shear strain at relatively high pressure promotes SC significantly.

2) If $M > 1$, even if the pressure for the initiation of SC can be reduced significantly because of strain-induced nucleation, only a small amount of product phase can be produced

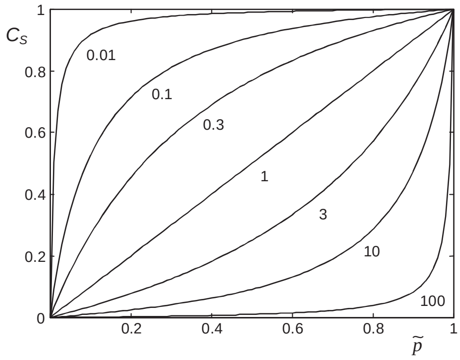

Fig. 2 – Relation between the stationary value of the volume fraction of the second phase and dimensionless pressure for $n = \zeta = 1$. Numbers near the curves designate values of M.

at a pressure around $p_\varepsilon^{\mathrm{d}}$. A significant amount of the product phase can be obtained under the pressure around $p_{\mathrm{h}}^{\mathrm{d}}$, *i.e.* as for pressure-induced SC.

A significant amount of high-pressure phase can be induced by a large strain at a low pressure for $M \ll 1$ only (fig. 2). One of the conditions for a small M, $(\sigma_{y2}/\sigma_{y1})^{w/g} \gg 1$, shows that large plastic strains promote the appearance of hard phases more than weak phases. When this condition is fulfilled, then plastic flow localizes inside of phase 1 causing $1 \rightarrow 2$ SC, while small plastic strain in phase 2 causes a small advance of the reverse SC.

3) For $p_\varepsilon^{\mathrm{d}} > p_\varepsilon^{\mathrm{r}}$, reverse SC does not occur for $p > p_\varepsilon^{\mathrm{d}}$ and complete SC is possible. In this case, the second term in the right-hand side of eq. (5) disappears and $c_{\mathrm{s}} = 1$. *E.g.*, graphite can be transformed (via amorphous carbon) to diamond at room temperature, $p = 19$–$25\,\mathrm{GPa}$ and shear strain of 0.2 [28]. However, reverse SC is practically impossible under such pressure because of the small plastic deformation which a diamond can experience.

4) Zero-pressure hysteresis was observed at pressure $p = 1.8\,\mathrm{GPa}$ for the $B1 \leftrightarrow B2$ transformation in KCl [11] and it was assumed that this was a phase equilibrium pressure. However, if the system is in a stationary state under any pressure p with $c = c_{\mathrm{s}}$, then any infinitesimal pressure increase (decrease) followed by plastic straining will cause $1 \rightarrow 2$ $(2 \rightarrow 1)$ SC, *i.e.* pressure hysteresis is zero. Equilibrium pressure p_{e} does not appear in any equation for the strain-induced SC and, consequently, cannot be determined from the strain-induced experiment.

Possible microscopic ways of controlling SCs. – One aim of controlling the strain-induced SCs, leading to high-pressure phases metastable at ambient pressure, is to decrease K_{d} and $p_\varepsilon^{\mathrm{d}}$ for direct SC and to increase K_{r} and reduce $p_\varepsilon^{\mathrm{r}}$ (or at least $p_{\mathrm{h}}^{\mathrm{r}}$) below atmospheric pressure. According to the equation $K = L\varepsilon_0\sigma_y(q)$ [21, 22], plastic strain leads to strain hardening and an increase in σ_y, K_{d}, and K_{r}, *i.e.* to an increase of pressure hysteresis for pressure-induced SCs. This explains why plastic straining under conditions which do not cause SC, substitutes reversible pressure-induced SCs with irreversible ones. For strain-induced SCs, the growth of K is more than compensated by an increase in the driving force due to the stress concentration at defects generated during plastic flow. That is why pressure hysteresis decreases. So, there is no contradiction between the results reported in [4, 11] and [12].

Annealing at a pressure below $p_\varepsilon^{\mathrm{d}}$ will reduce the yield stress σ_y, K_{d}, and $p_\varepsilon^{\mathrm{d}}$. Consequently, heating under pressure (or after intermediate unloading) can be used to further decrease pressure for the initiation of stress- and strain-induced SCs. Avoiding (minimizing) plastic straining at $p < p_\varepsilon^{\mathrm{d}}$ by choosing the proper loading history and sample, one can decrease K_{d}, and $p_\varepsilon^{\mathrm{d}}$ as well. Reduction of $p_{\mathrm{h}}^{\mathrm{r}}$ and $p_\varepsilon^{\mathrm{r}}$ can be achieved by a large plastic deformation of high-pressure phase at a pressure slightly above $p_\varepsilon^{\mathrm{r}}$ (to avoid strain-induced reverse SC). Another point is to find an unloading path, which minimizes or avoids plastic straining during unloading. Then one has to reduce $p_{\mathrm{h}}^{\mathrm{r}}$ below atmospheric pressure (rather than to worry about $p_\varepsilon^{\mathrm{r}}$ as well). *E.g.*, plastic deformation of the high-pressure phase II of Ge and Si by a rotation by 10° reduced transformation pressure to semiconducting phase III from 4.3 GPa to 2.3 GPa for Ge and from 4.7 to 2.7 GPa for Si [4]. One possible way to reduce plastic strain during unloading is to make unloading as fast as possible (quenching from a high-pressure state).

If alternative phases 2 and 3 can appear as a result of SC from phase 1, then the kinetic equation for the volume fraction of each phase has to take into account strain-induced direct and reverse SC of each phase into the other phases. Let $\sigma_{y\mathrm{w}} \ll \sigma_{y\mathrm{s}}$, where "w" designates weak and "s" strong. Note that for a stronger phase, $K = L\varepsilon_0\sigma_y$ is larger than for a weaker phase (assuming the same L and ε_0). That is why even if $p_{\mathrm{e}}^{1\rightarrow\mathrm{w}} > p_{\mathrm{e}}^{1\rightarrow\mathrm{s}}$, it may happen that $p_{\mathrm{h}}^{1\rightarrow\mathrm{w}} < p_{\mathrm{h}}^{1\rightarrow\mathrm{s}}$. Then the stronger phase cannot be obtained under hydrostatic loading. However, plastic straining promotes SC to a stronger phase. If a stronger phase appears, deformation is more concentrated in the parent phase, and $\frac{\sigma_{y\mathrm{s}}}{\sigma_{y1}} > \frac{\sigma_{y\mathrm{w}}}{\sigma_{y1}}$ in kinetic equations. If both the strong and weak phases appear, again deformation is more concentrated in the weaker phase which may cause SC w → s. As supporting examples, we can consider phase transformations in Ge and Si, for which a strong, semiconducting phase I can be transformed to a strong, semiconducting phase III or a weak, metallic phase II [4]. Despite the fact that $p_{\mathrm{e}}^{1\rightarrow\mathrm{w}} > p_{\mathrm{e}}^{1\rightarrow\mathrm{s}}$ for these materials, $1 \rightarrow \mathrm{w}$ transformation occurs under hydrostatic conditions, but $1 \rightarrow \mathrm{s}$ transformation does not. The rotation of the anvil leads to transformation from phase I to III instead of to the weaker phase II [4]. Consequently, the method based on the compression of materials with the rotation of an anvil is especially important for the search and production of high-strength materials.

The obtained equations also explain the results reported in [5, 6]. A matrix with a yield stress higher (lower) than that for reagents significantly promotes (suppresses) the reactions, because plastic strain is concentrated in the reacting material (matrix). Similarly, we can conclude that adding stronger particles to the material under study will facilitate SC and could cause SCs which were not obtained otherwise, *e.g.* metallic hydrogen [24–26]. Adding weaker particles will suppress SC, which is important, *e.g.*, for explosives.

One of the conclusions is that, to obtain SCs which are at the limit of current experimental ability (*e.g.*, [24–26]), one can substitute pressure-induced SC by strain-induced SCs using rotation of an anvil, as well as the above methods of intensification of strain-induced SCs. The above results will be qualitatively the same for any reasonable kinetic equation, because they are based on experimental and theoretical facts that direct and reverse strain-induced SCs can occur simultaneously, that there exist limiting pressures $p_\varepsilon^{\mathrm{d}}$ and $p_\varepsilon^{\mathrm{r}}$, and that strain in the weaker phase is larger than in the stronger phase.

Note that in most cases, even without the rotation of an anvil, when a high-pressure experiment is performed without hydrostatic media, the specimen undergoes large plastic deformations [14,24–26]. This is the case in experiments under megabar pressure, in particular, with solid hydrogen [24–26]. Transformation conditions for such a case are characterized by the pressure only (like for pressure-induced SC) and are compared with or led by atomistic calculations of phase equilibrium pressure. We believe that this is conceptually wrong, and even the term "pressure-induced SCs" is misleading in such a situation. This is even more true for the case with rotation of an anvil. The usual way of characterization (SC pressure at prescribed rotation or shear) is not complete. Strain-induced SCs under high pressure can be completely characterized by a strain-controlled kinetic equation of the type of eq. (5) only. This is conceptually similar to the characterization of strain-induced transformations in

TRIP steels at normal pressure. In contrast to our approach, the kinetic equation for TRIP steels [19, 20] is not thermodynamically derived and does not account for the reverse SC.

Preliminary values for some of the parameters for $B1 \leftrightarrow B2$ transformation in KCl are: $p_\varepsilon^{\mathrm{d}} = 1.25\,\mathrm{GPa}$, $p_{\mathrm{h}}^{\mathrm{d}} = 2.9\,\mathrm{GPa}$ (after large plastic straining), $\chi = 0.215$, and $a = 0.626$. The obtained kinetic equation (5) is currently used as a constitutive equation for the macroscopic model, more detailed than in [13, 14].

* * *

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