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# On the Taylor–Quinney coefficient in dynamically phase transforming materials. Application to 304 stainless steel

R. Zaera [a,*], J.A. Rodríguez-Martínez [a], D. Rittel [a,b]

[a] Department of Continuum Mechanics and Structural Analysis, University Carlos III of Madrid, 28911 Leganés, Madrid, Spain
[b] Faculty of Mechanical Engineering, Technion, 32000 Haifa, Israel

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ABSTRACT

We present a thermodynamic scheme to capture the variability of the Taylor–Quinney coefficient in austenitic steels showing strain induced martensitic transformation at high strain rates. For that task, the constitutive description due to Zaera et al. (2012) has been extended to account for the heat sources involved in the temperature increase of the material. These are the latent heat released due to the exothermic character of the transformation and the heat dissipated due to austenite and martensite straining. Through a differential treatment of these dissipative terms, the Taylor–Quinney coefficient develops a direct connection with the martensitic transformation becoming stress, strain and strain rate dependent. The improved constitutive description sheds light on experimental results available in the literature reporting unusual ($>1$) values for the Taylor–Quinney coefficient.



## 1. Introduction

Many advanced processes in engineering such as high-speed metal forming (Rojek et al., 2001), cutting (Miguélez et al., 2009; Molinari et al., 2010; Ma et al., 2012), crash in energy absorbing structures (Reyes et al., 2002; Rusinek et al., 2008) or impact on metallic plates (Rosenberg and Dekel, 2004; Rodríguez-Martínez et al. (2010a,b)) involve large strains at high strain rates. In these conditions, the thermodynamic process deviates from the isothermal state and approaches adiabaticity, leading to large and sometimes very rapid variations in the temperature field. The analysis should then use temperature-dependent mechanical properties where thermal softening of the material should be considered since dynamic plastic instabilities, such as adiabatic shear bands or necking, are known to be temperature dependent (Molinari, 1997; Bonnet-Lebouvier et al., 2002; Rodríguez-Martínez et al., 2010c).

The main source for temperature increase in the absence of external heat usually comes from plastic dissipation. In practice, a correct determination of this dissipation is needed for a proper evaluation of material softening in high strain rate applications. Following Tresca (1879), Farren and Taylor (1925) and Taylor (1934) were the first who observed that plastic work is not entirely converted into heat in the deformation of metals, so that part of it is stored in cold work – so-called stored energy of cold work – Bever et al. (1973). Following these seminal contributions, the Taylor–Quinney coefficient has been defined as the ratio of dissipated to plastic works (in its integral form $\beta_{int}$), or dissipated to plastic powers (in its differential form $\beta_{diff}$), as discussed by Rittel (1999). These coefficients are used to calculate the temperature increase in the simulation of dynamic processes. Here, it is important to note that the integral factor cannot exceed a value of 1 due to its very definition, a restriction that does not apply to instantaneous power ratios (Rittel, 1999).

* Corresponding author. Tel.: +34 916249983; fax: +34 916249430.
*E-mail address:* ramon.zaera@uc3m.es (R. Zaera).

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Different authors have measured these coefficients in polymers (Ravi-Chandar, 1995; Rittel, 1998; Bjerke et al., 2002) and metals (Mason et al., 1994; Chrysochoos et al., 1989; Kapoor and Nemat-Nasser, 1998; Hodowany et al., 2000; Oliferuk et al., 2004; Rittel et al., 2012) by using a variety of experimental techniques such as thermography, embedded thermocouples or high speed infrared detectors. For the sake of simplicity it is often assumed that the two $\beta$ factors are constant, usually taking a value lower than 1, or equal to 1 when all the plastic work is used to heat the material (Kapoor and Nemat-Nasser, 1998; Brünig and Driemeier, 2007; Baig et al., 2012; Khan and Liu, 2012). Once determined, they can be used in a model to calculate thermal output work as a fraction of the dissipated input plastic power. However, different authors reported a functional dependence of $\beta_{int}$ upon strain and/or strain rate (Bever et al., 1973; Mason et al., 1994; MacDougall, 2000; Rittel et al., 2006; Rusinek and Klepaczko, 2009; Rittel et al., 2012), a fact that may significantly complicate the solution of the coupled heat equation (Boley and Weiner, 1960).

When plastic deformation is governed by dislocation slip, this dependence has been explained through the effect of strain in the dislocation density increase and work converted into heat (Bever et al., 1973; Zehnder, 1991), as can be found e.g. in Benzerga (Benzerga et al., 2005). However additional processes may take place during plastic deformation, of which twinning is quite commonly observed, as a mechanism that stores little energy of cold work while contributing significantly to the strain hardening (Bever et al., 1973; Padilla et al., 2007; Osovski et al., 2012). Additional phenomena may be induced by high rate straining of crystalline solid like dynamic recrystallization (Khan et al., 2007; Rittel et al., 2008; Osovski et al., 2012; Cerreta et al., 2012; Brown and Bammann, 2012). Also during phase transformations such as the conversion of austenite to martensite, well known to occur in a reversible way in pure iron (Rittel et al., 2006) or to develop in many ferrous alloys such as metastable austenitic steels of the 3XX series (Rodríguez-Martínez et al., 2011) or with high manganese content. In such cases, the measured temperature rise comprises the effects of exothermal phase transformations during which latent heat is released. When this is the case, a simple ratio of the thermal to mechanical power and work, into which this extraneous heat source is included, may yield effective values of $\beta_{diff}$ and $\beta_{int}$ which exceed 1, as reported by Rittel et al. (2006) for pure iron, by Rusinek and Klepaczko (2009) for Transformation Induced Plasticity (TRIP) steels or by Jovic et al. (2006) for austenitic steels.

Considering specifically strain-induced phase transformations, the Strain Induced Martensitic Transformation (SIMT) is found e.g. in multiphase TRIP steels (Khan et al., 2012; Lim et al., 2012) and metastable austenitic grades (Lindgren et al., 2010; Kubler et al., 2011). These two alloys are frequently used by the industry for energy absorption in crash (Rodríguez-Martínez et al., 2010b; Andersson, 2005) or blast protection applications (Langdon and Schleyer, 2005a,b, 2006) due to their ductility and work hardening ability. This type of martensitic transformation occurs within a given range of temperatures $M_s^\sigma$ to $M_d$ covering the in-service conditions of TRIP and austenitic steels in many industrial applications. Above $M_s^\sigma$ the stress needed for martensite nucleation exceeds the flow stress of the austenitic phase, which should thus strain-harden to sustain martensite formation. As the temperature rises, austenite stability increases thereby limiting the transformation. Above $M_d$ martensite is not produced anymore (Lichtenfeld et al., 2006; Curtze et al., 2009).

Therefore a strong coupling is expected to exist between SIMT and heat generation in these alloys: SIMT contributes to heat through a latent heat term (exothermal transformation) and heat, in turn, hinders SIMT. Thus the latent heat released during martensitic transformation should modify the ratio of dissipated to plastic power. The weight of dislocation mediated (slip) plasticity in the inelastic deformation of the alloy should progressively decrease as austenite transforms into martensite, analogous to a twinned phase, thus leading to additional changes in the value of the stored energy of cold work. All these factors will most likely affect the value of the Taylor–Quinney coefficient upon deformation. However, this specific issue, barely reported in experimental work, has not been yet investigated and modeled systematically to the best of the authors' knowledge.

Therefore, we present a theoretical approach to evaluate the variability of the Taylor–Quinney coefficient in steels exhibiting SIMT. A constitutive model, previously proposed by Zaera et al. (2012) and now modified to account for the different heat rates, has been used. This model includes strain, strain rate and temperature effects in the phase transformation kinetics, and in the softening of each solid phase through the use of a homogenization technique. The model also allows considering the influence of stress state in the SIMT (Young, 1988). This work considers AISI 304 stainless steel, a reference metastable austenitic stainless steel for studying the SIMT process at high strain rates since it shows a large amount of transformed martensite even under adiabatic conditions (Rodríguez-Martínez et al., 2011). The new model sheds light on previous experimental results reporting unusual ($> 1$) values for the Taylor–Quinney coefficient (Rittel et al., 2006; Jovic et al., 2006; Rusinek and Klepaczko, 2009), apparently related to an exothermal phase transformation, through a differential treatment of the dissipative terms, namely latent heat and heat due to austenite and martensite plastic deformation. Likewise the model accounts for the strong coupling existing between martensitic transformation, strain, strain rate, stress state and heat release, thus allowing to perform a thorough analysis of their influence in the evolution of the ratio of dissipated to plastic power and work. The variability observed in $\beta_{diff}$ and $\beta_{int}$ shows the inherent limitations of assuming a constant value of the Taylor–Quinney coefficient when modeling high strain rate problems in alloys showing SIMT. On the contrary, taking into account the functional dependence of $\beta_{diff}$ and $\beta_{int}$ avoids considering an averaged value which may either under- or over-estimate the heat dissipated during the deformation process.

The paper is organized as follows. Section 2 shows the new thermodynamic approach proposed to calculate the variable Taylor–Quinney coefficient, highlighting the differences with the standard approach which considers a constant value. Section 3 provides a brief summary of the thermoviscoplastic constitutive equations used to model the SIMT. Section 4 describes the different finite element models developed to perform the study. In Section 5 the set of equations is integrated and the