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A Uniaxial Nonlinear Tension-Compression Constitutive Model Based on Boltzmann Function for Typical PBXs under Quasi-Static Loading

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Abstract: In the tension and compression tests under quasi-static loading, almost all polymer bonded explosives (PBXs) reflect obviously nonlinear constitutive behavior, now commonly used constitutive model in the description of the nonlinear adaptability is not ideal. Aimming at the nonlinearity and asymmetry of stress-strain curves for five typical PBXs (PBX-X, PBX-9502, LX-17, PBX-9501, and EDC-37), a quasi-static constitutive model with four parameters that considers both tension and compression was deduced based on Boltzmann function. Based on the discussion of the physical meaning of undetermined parameters for the model, on account of determined method of undetermined parameters proposed in this paper, the stress-strain curves for five kinds of typpical PBXs were fitted by the constitutive model. Results show that the constitutive model can well describe the constitutive behavior at different temperatures and strain rates for typpical PBXs. The constitutive model of tension and compression based on the Boltzmann function is expected to be widely used as a universal quasi-static constitutive model for different PBX materials.

Key words: polymer bonded explosive(PBX); stress-strain curve; constitutive model; Boltzmann function

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1 Introduction

Polymer bonded explosives (PBXs), a kind of energetic material, are mainly composed of explosive crystal, polymer, plasticizer, and desensitizer. The mass ratio of explosive crystal is often more than 90%. Except for energy supply, PBXs in weapon systems also have to bear thermal-mechanical loads during assembly, transportation, storage and usage. Damaged explosive parts may induce danger and affect the propagation of detonation waves[1]. Constitutive model is the basis to study the mechanical behaviors of materials, and it plays an important role in evaluating the mechanical response of structural components in service environment, especially in simulation code for engineering analysis.

The constitutive response of PBXs is very complex to model because of the nonlinearity and asymmetry of their stress-strain curves. In 1984, a constitutive model of PBX was established by Browning et al[2]. This model was developed in 1989, but it is a one-dimensional model[3]. The one known as the ViscoSCRAM[3] is the most famous model for PBXs in recent years, and it is still working now according to the studies[4-5] of Los Alamos National Laboratory (LANL). It is based on capturing time-dependent behavior by combining a viscoelastic model with the accumulation of internal damage. Actually, the ViscoSCRAM model could not fit the test results well now[6-7], because its parameters are difficult to confirm. Moreover, although many studies on stress-strain curves of typical PBXs have been reported[8-11], no research has studied the universal constitutive model of explosive materials considering both tension and compression. Normally, tension and compression are studied independently, and the tensile curve at room temperature is often viewed as linear[12-13]. As a result, the calculation process may go against with practical behaviors and cause errors. There are certainly many other investigations[14-15] about this relationship, but just like what Devin Shunk said in his report[16], even with all of the exploratory work, the constitutive models for PBXs are still lacking. Thus, Boltzmann function is proposed in this paper to establish a uniaxial nonlinear constitutive model for typical PBXs under quasi-static loading, both tension and compression were considered in the model.

2 Modeling

2.1 Mechanical Properties of Typical PBXs

PBX-X, PBX-9502, LX-17, PBX-9501, and EDC-37 are

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five typical PBXs of different countries, their names and components are listed in Table 1. The stress-strain curves of Chinese PBX-X in present paper have similar common features with the rest four, and they are obtained by universal testing methods. A typical stress-strain curve of PBX-X, including both tension and compression data at 50 ℃, is shown in Fig. 1. The curves are typically S-shaped with obvious nonlinearity. The modulus decreases gradually with load increasing. Moreover, the curve also shows obvious asymmetry by the absence of a plateau when the material is under tension. After the maximum compression stress is reached, the stress gradually decreases with the strain increasing continuously until a sudden failure happens to the material.

Table 1 Information of the five PBXs

nation	name	explosive crystal mass fraction	binder major components
China	PBX-X	>94% TATB	fluoro rubber
America	PBX-9502	95% TATB	Kel-F800
America	LX-17	92.5% TATB	Kel-F800
America	PBX-9501	95% HMX	estane + BDNPA-F
United Kingdom	EDC-37	91% HMX	K-10 + nitrocellulose

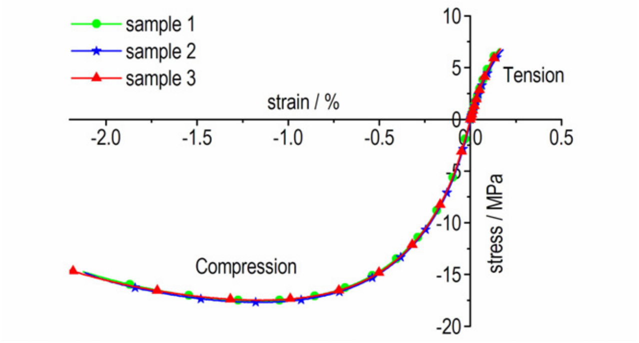


Fig. 1 Tension-compression stress-strain curves of China's PBX-X at 50 ℃

2.2 Theoretical Analysis

From Fig. 1, we know that the typical stress-strain behaviour of PBXs is an S-shaped curve with nonlinearity and asymmetry. As typical S-shaped curve functions, Boltzmann sigmoid, Gaussian cumulative, and Lorentz cumulative are commonly used to describe the transition behavior of some physical quantities, and they have been widely applied in the fields of medicine, biology, agriculture, physics, and chemistry[17-18]. Their mathematical expressions[18] are given in Eqs. (1), (2) and (3), respectively:

$$y(x)=\frac{Y_1-Y_2}{1+e^{(x-x_0)/dx}}+Y_2 \qquad (1)$$

$$y(x)=\frac{(Y_2-Y_1)\arctan(((x-x_0)/dx)+(\pi/2))}{\pi}+Y_1 \qquad (2)$$

$$y(x)=\frac{Y_2-Y_1}{2}\left(1+\frac{2}{\sqrt{\pi}}\int_0^{\frac{x-x_0}{\sqrt{2}dx}}e^{-t^2}dt\right)+Y_1 \qquad (3)$$

The physical significance of each parameter in theseEqs is the same: x is the independent variable, whereas y is the dependent variable. Four undetermined coefficients are used: Y_1 and Y_2 are the theoretical lower limit and upper limit of function y, respectively; x_0 is the midpoint of x; and dx is used to represent the degree of curve changes. The rate of curve at x_0 is proportional to $1/dx$. All of the three functions describe the S-shaped curve shown in Fig. 2 in different mathematical forms.

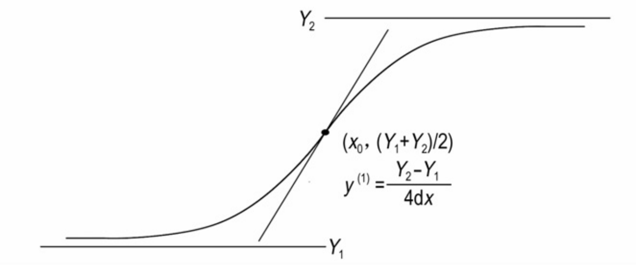


Fig. 2 Typical S-shaped curve and physical significance of parameters

When y denotes stress and x denotes strain, Boltzmann sigmoid, Gaussian cumulative, and Lorentz cumulative can be used as the mathematical expressions of the constitutive model of materials with an S-shaped stress-strain curve. Given that these functions describe the curve of same type, the Boltzmann function, which is the simplest one, is adopted in this work to describe the constitutive model of PBXs. The Boltzmann function, which considers both tension and compression, conforms to the mathematical characteristics of PBXs' stress-strain curves. More importantly, it is convenient to determine the values of undetermined coefficients, because their physical significance is relatively definite. The constitutive model based on the Boltzmann function could be expressed as:

$$\sigma=\frac{\sigma_{ccs}-\sigma_{tcs}}{1+e^{\alpha\varepsilon+\beta}}+\sigma_{tcs} \qquad (4)$$

where σ and ε are the stress (MPa) and strain (dimensionless factor), respectively (positive in tension and negative in compression); the four undetermined coefficients, namely, σ_{ccs}, σ_{tcs}, β, and α are the theoretical lower and upper limits of stress (MPa) correction factor of stress-strain at zero point (dimensionless factor) and the modulus correlation coefficient (dimensionless factor), respectively. The initial values can be determined via the following method:

(1) σ_{ccs} and σ_{tcs} are the compressive and tensile critical stresses, respectively. For ductile materials with evident tensile and compressive plateau in stress-strain curves, the values of σ_{ccs} and σ_{tcs} are the compressive and tensile strengths. Given

the brittle nature of PBXs, only the compressive plateau is observed (i. e., no tensile plateau). The value of σ_{ccs} is the compressive strength. The initial value of σ_{tcs} is larger than its tensile strength. It is an infinite virtual value and is inversely proportional to the compressive strength.

(2) The physical significance of β, the correction coefficient of the stress-strain at zero point, is that when the strain is zero, the stress is also zero. This relationship is the basic attribute of the quasistatic constitutive model. When zero strain and zero stress are substituted into Eq. (4), Eq. (5) can be obtained. Particularly, if the tensile stress-strain curve and compressive stress-strain curve are perfectly symmetrical and the absolute values of σ_{ccs} and σ_{tcs} are equal, then $\beta=0$.

$$e^{\beta}=-\frac{\sigma_{ccs}}{\sigma_{tcs}}\Leftrightarrow\beta=\ln\left(-\frac{\sigma_{ccs}}{\sigma_{tcs}}\right) \qquad (5)$$

(3) The mathematical expression of the modulus [Eq. (6)] can be obtained from Eq. (4). The modulus is a variable that changes with strain, and its maximum value is achieved at the zero strain point. At this point, Eq. (7) is the mathematical expression of the modulus correlation coefficient α. When the elasticity modulus E_0 close to the zero point is substituted into Eq. (7), the initial value of α can be determined. Particularly, when $\beta=0$, Eq. (7) can be simplified into Eq. (8).

$$E=\frac{d\sigma}{d\varepsilon}=-\frac{\alpha e^{\alpha\varepsilon+\beta}(\sigma_{ccs}-\sigma_{tcs})}{(1+e^{\alpha\varepsilon+\beta})^{2}} \qquad (6)$$

$$E_0=\frac{\alpha e^{\beta}(\sigma_{tcs}-\sigma_{ccs})}{(1+e^{\beta})^{2}}\Leftrightarrow\alpha=\frac{E_0(1+e^{\beta})^{2}}{e^{\beta}(\sigma_{tcs}-\sigma_{ccs})} \qquad (7)$$

$$E_0=\frac{\alpha(\sigma_{tcs}-\sigma_{ccs})}{4}\Leftrightarrow\alpha=\frac{4E_0}{\sigma_{tcs}-\sigma_{ccs}} \qquad (8)$$

3 Results and Discussion

This Boltzmann function based nonlinear tension-compression constitutive model is described as Eq. (4), its initial values of the parameters are determined via test data and the methods introduced above. Finally, the test data[8-11] and fitting curves of PBX-X, PBX-9502, LX-17, PBX-9501, and EDC-37 are shown in Fig. 3 and Fig. 4, respectively. The testing temperature and strain rate, as well as the fitting results and its applicable range, are listed in Table 2. All of the values of the adjusted R-square are higher than 0.99, thereby the fitting results of both the 1, 3, 5-triamino-2, 4, 6-trinitrobenzene (TATB)-based PBXs (PBX-901, PBX-9502, and LX-17) and

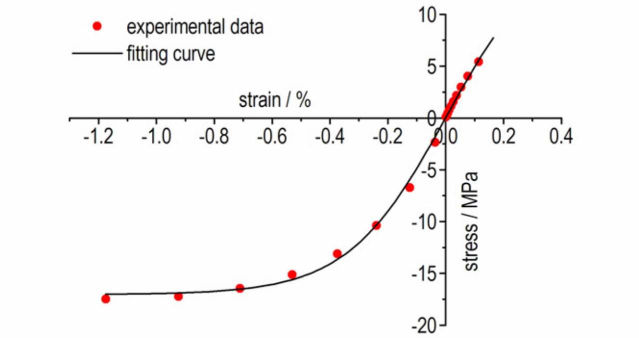
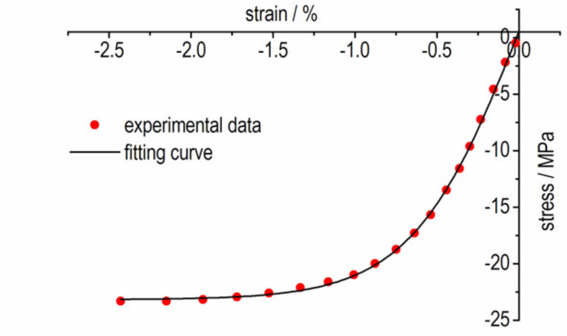
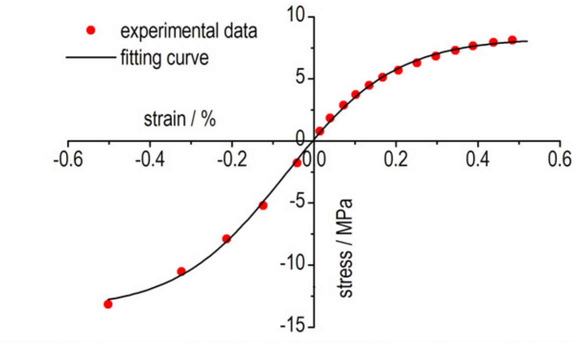


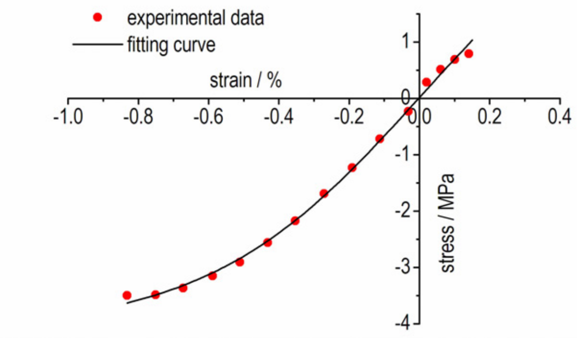
Fig. 3 Experimental data and fitting curve for PBX-X at 50 ℃



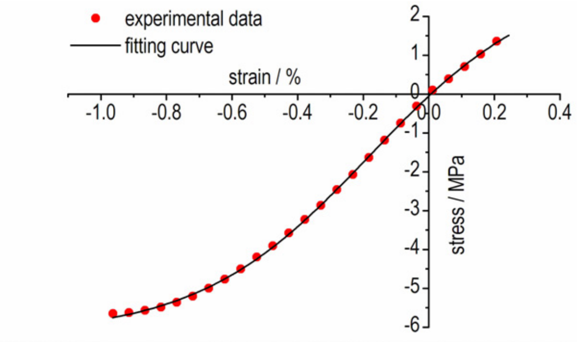
a. PBX-9502 at 20 ℃



b. LX-17 at 22 ℃



c. PBX-9501 at 50 ℃



d. EDC-37 at 20 ℃

Fig. 4 Experimental data and fitting curves for PBX-9502, LX-17, PBX-9501 and EDC-37 octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX)-based PBXs (PBX-9501 and EDC-17) are satisfying. The Boltzmann function based constitutive model can be widely used in different PBX materials.

Additionally, the above test data of PBX-X is obtained from laboratory test, and the rest data is collected from literatures. In practical engineering, the mechanical behaviors of explosive structural components are calculated and predicted via numerical simulation. The constitutive model is required to describe the stress-strain relationship precisely at least in the zone from the maximum compressive stress to the maximum tensile stress, which can be satisfied by the Boltzmann function used above. However, the region from the maximum compression stress to the sudden failure cannot be described mathematically by the established constitutive model yet.

Table 2 Constitutive model parameters for the five PBXs

type	T/℃	strain rate	σ_{ccs}/MPa	σ_{tcs}/MPa	β	α	strain range/%	R^2
PBX-X	50	4.17×10^{-4}	−17.039	17.118	-4.626×10^{-3}	5.896	(−1.175, 0.165)	0.99791
PBX-9502	20	8.30×10^{-4}	−23.184	25.147	-8.128×10^{-2}	3.029	(−2.428, 0.000)	0.99927
LX-17	22	1.25×10^{-5}	−13.559	8.293	4.916×10^{-1}	7.583	(−0.502, 0.520)	0.99898
PBX-9501	50	1.00×10^{-5}	−4.118	4.149	-7.500×10^{-3}	3.327	(−0.832, 0.151)	0.99789
EDC-37	20	4.00×10^{-5}	−6.192	3.030	7.147×10^{-1}	3.828	(−0.963, 0.244)	0.99977

4 Conclusions

(1) The uniaxial quasi-static tension-compression stress-strain curves of PBXs have evident nonlinearity, and these curves have poor asymmetry and exhibit a typical S-shape.

(2) Boltzmann function is a widely used typical S-shaped curve function, the constitutive model deduced based on the Boltzmann function has four undetermined coefficients (namely, the theoretical lower limit of stress, the theoretical upper limit of stress, correction factor of stress-strain at zero point and the modulus correlation coefficient.), their initial values can be determined by theoretical analysis without fitting.

(3) The uniaxial nonlinear constitutive models of five typical PBXs (PBX-X, PBX-9502, LX-17, PBX-9501, and EDC-37) were established according to their stress-strain curves. The values of the adjusted R-square are higher than 0.997, it indicated that this constitutive model based on Boltzmann function is capable of describing the stress-strain relationship at different temperatures and strain rates, and it can be widely used in different PBX materials as a universal constitutive model, in which both tension and compression nonlinearity are considered.

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典型 PBX 基于 Boltzmann 函数的准静态单轴拉压非线性本构模型

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摘 要：准静态载荷下的拉伸压缩试验中，几乎所有高聚物粘结炸药（PBX）都体现出了明显的非线性本构行为，现常用的本构模型在描述这种非线性时适应性不甚理想。针对五种典型 PBX 炸药（PBX-X，PBX-9502，LX-17，PBX-9501，EDC-37）应力应变曲线的非线性及非对称性，基于 Boltzmann 函数推导了一种拉伸和压缩一起考虑的准静态单轴非线性四参数本构模型。在讨论模型待定参数物理意义的基础上，基于文中提出的待定参数初值确定方法，采用该本构模型对五种典型 PBX 的应力应变曲线进行了拟合。结果表明，该本构模型可较好地描述五种典型 PBX 炸药不同温度和应变率下的本构行为。基于 Boltzmann 函数的拉压非线性本构模型，有望作为一种适用于不同 PBX 的通用准静态本构模型广泛运用。

关键词：高聚物粘结炸药（PBX）；应力应变曲线；本构模型；Boltzmann 函数

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