Numerical simulation of Thermoelectric System

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Abstract: - The thermoelectric systems have attracted renewed interest as concerns with the efficient use of energy resources, and the minimization of environmental damage, have become important current issues. There has been he recognition that thermoelectric devices could play a role in generating electricity from waste heat, enabling cooling via refrigerators with no moving parts, and many other more specialized applications. This paper presents of numerical simulation for several the thermoelectric materials. Numerical simulation is carried out by using a finite element package ANSYS.

Key-Words: - numerical simulation, Peltier cooling, materials properties, temperature, voltage, figure of merit.

1 Introduction

The thermoelectric systems have been the subject of major advances in recent years, due to the development of semiconductors and the incorporation of the thermoelectric devices into domestic appliances. Generally, if a thermal gradient is applied to a solid, it will always be accompanied by an electric field in the opposite direction. This process is called as the thermoelectric effect. Thermoelectric material applications include refrigeration or electric power generation. The efficiency of a thermoelectric material is given by the figure of merit, Z, which is defined as [1]:

$$Z = \frac{\alpha^2 \cdot \sigma}{k}, \left[\frac{1}{K}\right] \tag{1}$$

where:
α - material's Seebeck coefficient, V/K,
σ - electrical conductivity of material, S/m,
k – thermal conductivity of material, W/(m·K).
The numerator in equation (1) is called the power factor. Therefore, the most useful method in order to describe and compare the quality and thermoelectric efficiency of different material systems is the dimensionless figure of merit (ZT), where T is the temperature of interest. Therefore, equation (1) can be rewritten as:

$$ZT = \frac{\alpha^2 \cdot \sigma \cdot T}{k} \tag{2}$$

An important point it is represented by achieving a high value of ZT, this being carried out by increasing the power factor ($\alpha^2\sigma$) and decreasing the thermal conductivity (k).
One of the main applications of thermoelectric is for refrigeration purposes. An electrical current applied across a material will cause a temperature differential which can be used for cooling [1].

2 Problem's definition

Consider the one dimensional $\left(\nabla = \frac{d}{dx}\right)$ steady-state, thermoelectric power generation problem, where only a single (n-or p-type) leg is considered. The thermoelectric material properties all vary with absolute temperature T. Positive electric current density and heat flux flows from T_h to T_c. Positive electric field E and temperature gradient are in the opposite direction of J and Q (Fig.1). The electric current density is for a simple generator, given by [2]:

$$J = \frac{I}{A} \tag{3}$$

where I is the electric current and A is the cross-sectional area of the thermoelectric element.

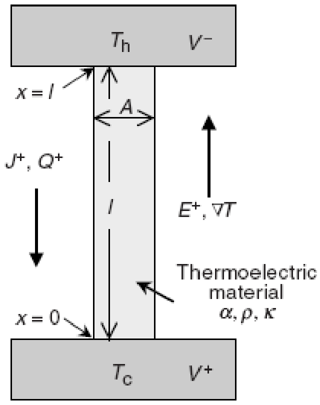

Fig.1 Diagram of a single-element thermoelectric generator (Source:[2])

The direction of positive variables is shown relative to the hot-and cold side. For positive Seebeck coefficient ($\alpha>0$), all of the variables are positive for a generator operating efficiently. For negative Seebeck coefficient ($\alpha<0$), the electric current, field and potential (J, E, V) will be negative or opposite to the direction shown [2].

The electric field is given by a combination of the reversible Seebeck effect and the irreversible effect of Ohm's law. Using the sign convention described above, the electric field from a purely resistive element using Ohm's law is $E = -\rho J$. The electric field produced by the Seebeck effect is $E = \alpha \nabla T$. Combining the Seebeck and Ohm effects, gives the electric field at any position:

$$E = \alpha \nabla T - \rho J \tag{4}$$

Similary, heat is transported reversibly by the Peltier effect, $Q = \alpha T J$, where αT is the Peltier coefficient and irreversibly by Fourier's law $Q = k \nabla T$, using sign convention of Fig.1:

$$Q = \alpha T J + k \nabla T \tag{5}$$

The Peltier effect is often considered a surface effect between two materials but the heat transported is a property of a single material [2]. In both cases (equation 4 and equation 5), the irreversible and reversible effects are treated independently, and can simply be summed. This treatment is related to Kelvin's assumption. The irreversible heat flow is further constrained by the steady-state heat equation:

$$\nabla(k \nabla T) = -T \frac{d\alpha}{dT} J \nabla T - \rho J^2 \tag{6}$$

where $T \frac{d\alpha}{dT}$ is the Thomson coefficient.

The electric power density P (power produced per volume) is the product of the electric field E and current density J:

$$P = EJ \tag{7}$$

Using sign convention in Fig. 1, a purely resistive element ($\alpha=0$) would require a negative electric field $E = -\rho J$ to make a positive current ($+J$) so that the power density $P = -\rho J^2$ is negative (electric energy consumed).

3 Design optimization

The performance of a thermoelectric generator is dependent on many variables that could be optimized globally to find the optimum design. However, by using a reduced variable approach to the design problem, many interdependencies of the design variables are eliminated, which allows a better understanding of the effect of each variable [2].

The first goal of the design process is to evaluate the highest possible thermoelectric efficiency for all hot-and cold-side temperatures (of the thermoelectric generator, not the heat sinks), which may be viable. This will produce an optimized efficiency that is only a function of the thermoelectric hot- and cold-side temperatures:

$$\eta = \eta_{\max}(T_h, T_c) \tag{8}$$

The presumption is that any other variables (such as materials chosen, interface temperatures, geometry, current, etc.) that may be required for the calculation of efficiency can be optimized given a T_h and T_c. This is true for the thermoelectric material interface temperatures, but less true for size of metal interconnect and contact resistance [2].

3.1 Thermoelectric Element Length

Once the optimized efficiency (equation 8) is found given a T_h and T_c, the values of $u(T)$ and $\Phi(T)$ for both the n- and p-element are defined. Most of the remaining performance parameters also require the thermoelectric element length. This is usually determined by the desired total heat flux $U_{total,h}/A_{total}$ (or power/area W/A_{total}). In order to calculate l and further operating conditions, the total heat flux $U_{total,h}/A_{total}$ or power/area desired W/A_{total} must be given. Thus, l is a function only of T_h, T_c, and $U_{total,h}/A_{total}$:

$$l = l\left(T_h, T_c, U_{total} / A_{total}\right). \qquad (9)$$

Once functions equation 8 and equation 9 are evaluated for a variety of T_h, T_c, and $U_{total,h}/A_{total}$, they can be incorporated into the system model to find the optimal system operation condition [2].
The system power and voltage are directly proportional to the size of the generator (through A_{total}) and number of couples. Once the system trades are complete, the final configuration of the thermoelectric generator can be established.

3.2 Voltage

The voltage produced V_{system} is the number of couples connected in series N_{series} times the couple voltage V_{couple} [2]:

$$V_{system} = V_{couple} N_{series}. \qquad (10)$$

Thus, the number of couples in series is determined by the voltage requirement. Often redundancy is desired by including additional parallel circuits $N_{parallel}$:

$$N_{system} = N_{series} N_{parallel}. \qquad (11)$$

Once the thermoelectric length is fixed, the total power desired W will define the total cross-sectional area A_{total}. The relationship between the area of a couple and the number of couples N_{system}, is given by:

$$A_{couple} = \frac{W}{\frac{U_{total}}{A_{total}} \eta N_{system}}. \qquad (12)$$

3.2 Temperature

Materials and device characterization play a key role in thermoelectric research. Materials composition and parameters affect the achieved thermoelectric (TE) performance (for example, functional properties and figure-of-merit of materials, efficiency, coefficient of performance, or sensitivity of devices).
As it is known, metals are poor thermoelectric materials because they have a low Seebeck coefficient and large electron contribution to thermal conductivity k, so electrical conductivity σ and thermal conductivity k will cancel each other out. A low thermoelectric effect is carried out by insulators which have a high Seebeck coefficient and small electron contribution to thermal conductivity, so their charge density and electrical conductivity are low. The best thermoelectric materials are between metals and insulators (i.e., semiconductors) [2], [3].
The thermoelectric materials of choice for the steady-state simulations illustrated in this paper on a thermoelectric element Peltier cooler are Bismuth-Tellurium (Bi-Te) and Lead-Tellurium (Pb-Te). They have a high Seebeck coefficient α, a good electric conductivity σ, and a poor thermal conductivity k.
Usually, those material properties depend on the temperature and may be anisotropic. Here only isotropic material properties are used at constant material parameters. Thermoelectric (TE) materials based on $(Bi,Sb)_2(Te,Se)_3$ are the best and, in fact, the only materials used for cooling. These include bismuth-tellurium (Bi-Te) and antimony-tellurium (Sb-Te) compounds. More recently, nanostructured materials have been investigated as candidates to increase the performance of thermoelectric devices. PbTe nanocomposites have been prepared from PbTe nanocrystals, synthesized via chemical route, by compaction under high pressure and temperature. The thermoelectric (TE) properties are found to vary with the shape and size of the composites' nanostructures. Transport properties of PbTe nanocomposites have been evaluated through temperature-dependent electrical conductivity, Seebeck coefficient, room temperature, and thermal conductivity measurements [4], [5].

4 Numerical simulation

Numerical simulation is carried out by using a finite element package ANSYS. This package operates with three stages: preprocessor, solver and postprocessor. The procedure for doing a static thermoelectricity analysis consists of following main steps: create the physics environment, build and mesh the model and assign physics attributes to each region within the model, apply boundary conditions and loads (excitation), obtain the solution, review the results.
In order to define the physics environment for an analysis, it is necessary to use the ANSYS preprocessor (PREP7) and to establish a mathematical simulation model of the physical problem [6].
In order to do this, the following steps are presented below: set GUI Preferences, define the analysis title, define element types and options, define element coordinate systems, set real constants and define a system of units, define material properties. ANSYS includes three elements which can be used in modeling the thermoelectricity phenomenon [6]. Element types establish the physics of the problem domain. Depending on the nature of the problem, it is

necessary to define several element types to model the different physics regions in the model.

A simple cooler geometry consists of one p-type semiconductor element 1x1x5.8mm³ in size [7]. It is contacted by two copper electrodes 0.1 mm in thickness (Fig.2).

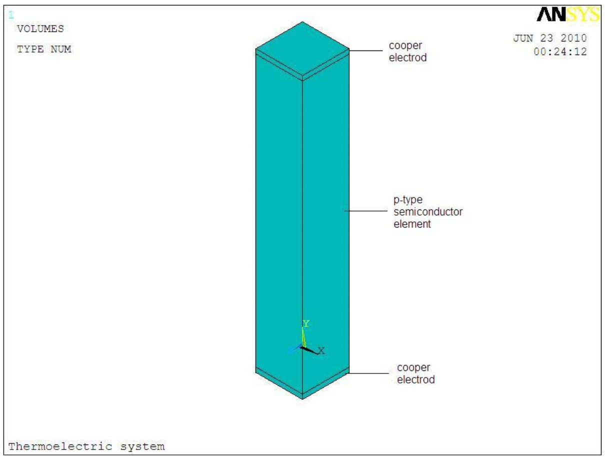

Fig.2 The model geometry for p-type thermoelectric leg

In the present application, for modeling the electric and thermal fields the SOLID227 element was chosen. SOLID227 has the following capabilities: structural-thermal, piezoresistive, electroelastic, piezoelectric, thermal-electric, structural-thermoelectric, thermal-piezoelectric [5], [8].

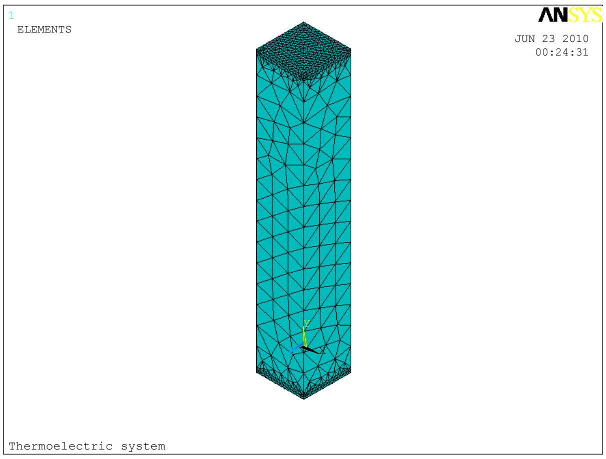

Fig.3 The mesh model with triangular elements

The element has ten nodes with up to five degrees of freedom per node. Thermoelectric capabilities include Seebeck, Peltier, and Thomson effects, as well as Joule heating.

Next step in the preprocessor phase is mesh generation and load application on the elements. It was used a mesh with 13711 nodes and 8586 triangular elements. The finite element mesh of the thermoelectric element is shown in Fig.3.

Table 1. Numerical material properties from [4], [7]

Material properties from	**Units measure**	**Bismuth-Tellurium (Bi-Te)**	**Lead-Tellurium (Pb-Te)**	**Cooper**
Seebeck Coefficient	α [V/K]	p:200e^{-6} n:-200e^{-6}	p:175e^{-6} n:-175e^{-6}	6.5e^{-6}
Electric resistivity	ρ [S/m]	0.9 e^{-5}	0.8 e^{-5}	0.169 e^{-8}
Thermal conductivity	λ [W/(mK)]	1.6	1.548	350
Density	δ [kg/m^3]	7740	8160	8920
Heat capacity	C [J/(kgK)]	154.4	156	385

The following examples show results of calculations for typical thermoelectric applications. The material properties for the calculations with temperature-independent values are shown in Table 1. Here typical values for Bismuth-Telluride, Lead-Telluride and copper were taken from [7].

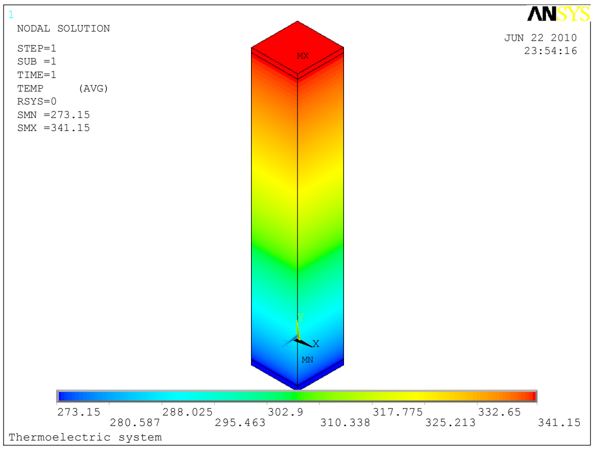

Fig.4 Distribution of temperature for Bi_2Te_3 material

A calculation model that simulates the thermal and electric performance of whole cooling based on thermoelectric technology has been implemented.

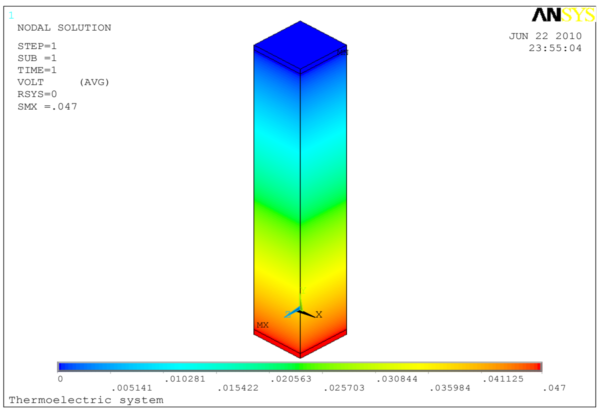

Fig.5 Distribution of voltage for Bi_2Te_3 material

The model inputs are: semiconductor materials and geometry, Peltier pellet components type, electrical voltage supplied to the Peltier pellet components and the hot and cold side temperatures.
The distribution of temperature for Bi_2Te_3 material is shown in Fig.4 and the distribution of voltage for Bi_2Te_3 material is shown in Fig.5.
When an electric current is running from the cold end to the hot end, the Joule heating is generated uniformly inside the element. The dissipated heat must reach both ends equally by conduction.
The cooler with Bi_2Te_3 material is designed to maintain the cold junction at a temperature T_c=273.15K and to dissipate heat from the hot junction T_h=341.15K.
Adiabatic boundary conditions were taken on all other surfaces. At the top of the upper electrode a current of 0.535A was applied.

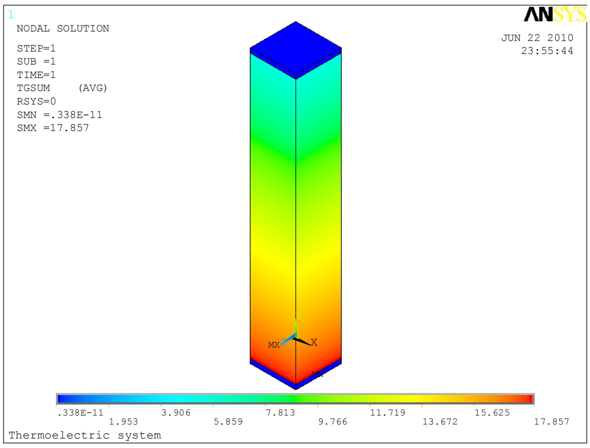

Fig.6 Distribution of thermal gradient for Bi_2Te_3 material

When a current passes through a material submitted to gradient of temperature, then the material exchanges heat with the outside medium.

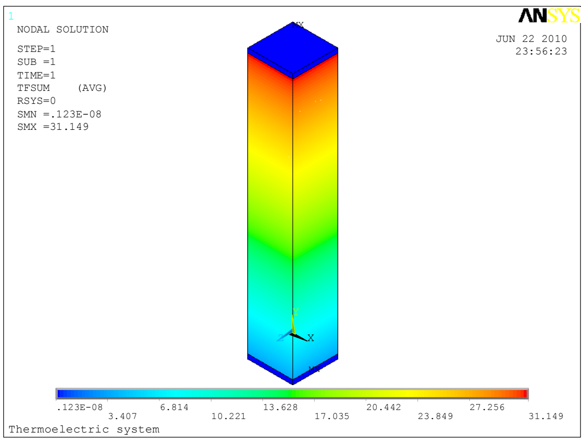

Fig.7 Distribution of thermal flux for Bi_2Te_3 material

Conversely, a current is produced when a heat flux passes through a material submitted to a temperature gradient.
In the case of cooling, the load is replaced by a dc-current source, which cases the charge carries to move from the cold zone to the hot zone. This implies a thermal flux opposite to the normal heat conduction.
After the simulation, the model-returned outputs are: temperatures, heat flows, thermal gradient, thermal flux, and voltage distribution. The distribution of thermal gradient for Bi_2Te_3 material is shown in Fig.6 and the distribution of thermal flux for Bi_2Te_3 material is shown in Fig.7.
The distribution of temperature for PbTe material is shown in Fig.8. The distribution of voltage for PbTe material is shown in Fig.9.

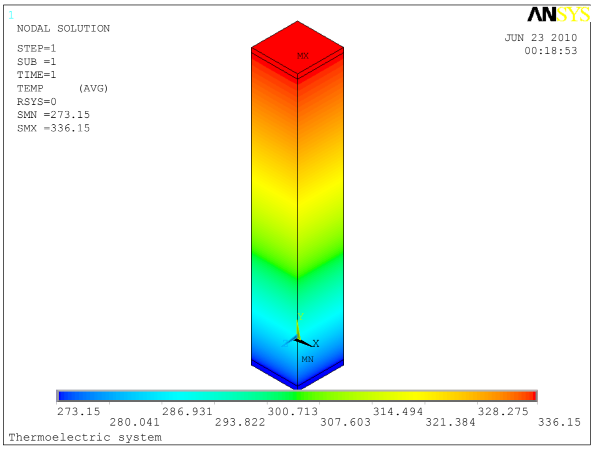

Fig.8 Distribution of temperature for PbTe material

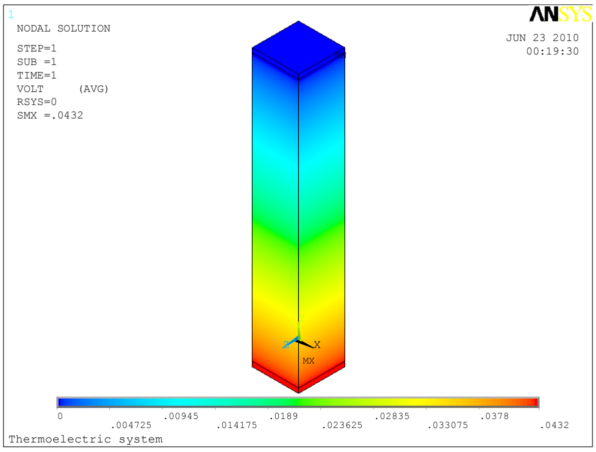

Fig.9 Distribution of voltage for PbTe material

The temperature dependence of Seebeck coefficient, electrical conductivity and power factor of the PbTe material lie within the temperature range 400–600 K.
Thermal conductivity reduction has played a central role in improving the thermoelectric figure-of merit,

ZT, of materials that already have a good power factor.

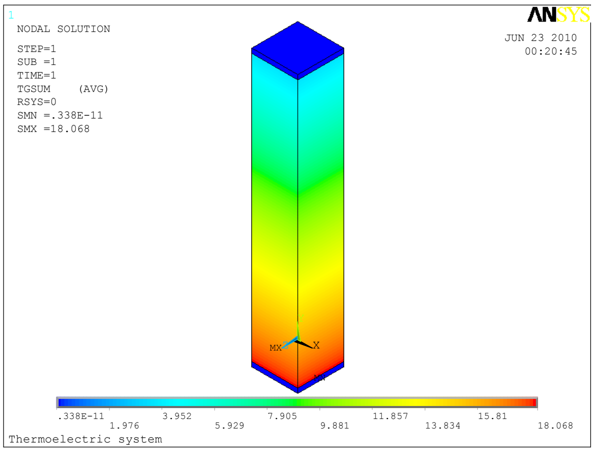

Fig.10 Distribution of thermal gradient for PbTe material

The distribution of the thermal gradient for PbTe material is shown in Fig.10 and the distribution of thermal flux for Bi-Te material is shown in Fig.11.

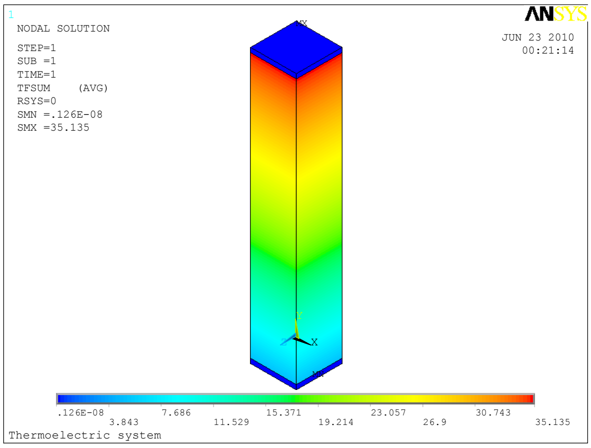

Fig.11 Distribution of thermal flux for PbTe material

When lead telluride PbTe is compared with bismuth telluride Bi_2Te_3, a temperature difference of nearly 63 K for cooler with PbTe and temperature difference of nearly 68 K for cooler with Bi2Te3 is noted. The voltage at the upper electrode is 47 mV for cooler with Bi_2Te_3 and 43.2 mV for cooler with PbTe. This means that, although the value of the figure of merit of PbTe is lower than for Bi_2Te_3, the latter material is used.

5 Conclusions

To calculate the exact performance of a thermoelectric devices analytically, it is simplest to use a reduced variables approach that will separate the intensive properties and variables (such as temperature gradient, Seebeck coefficient, current density, heat flux density) from the extensive ones (e.g., voltage, temperature difference, power output, area, length, resistance, load resistance). This approach allows a definition of a local, intensive efficiency in addition to the traditional system efficiency as well as the derivation of the compatibility factor.

Applications of the two materials Bi_2Te_3 and PbTe demonstrate the Peltier effect for thermoelectric cooling. It can be seen that a smaller thermal conductivity will decrease the heat transfer between the two ends, a smaller electrical resistivity will reduce the Joule heating, and a larger Seebeck or Peltier coefficient will enhance the heat removal. For most metals, the thermal conductivity is too high and the Seebeck coefficient is too small for refrigeration applications.

In fact, lead telluride-based materials have been used for a range of purposes in the hot-junction temperature range 600 to 900 K [2]. Conversely, PbTe has been considered more as a material for thermoelectric generation at moderately high temperatures rather than for refrigeration at room temperature and below [3]. PbTe thermoelectric generators have been widely used by the US army, in space crafts to provide onboard power, and in pacemaker batteries. The application shown in this paper can be useful to represent the characteristics of the Peltier cooling through numerical models.

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